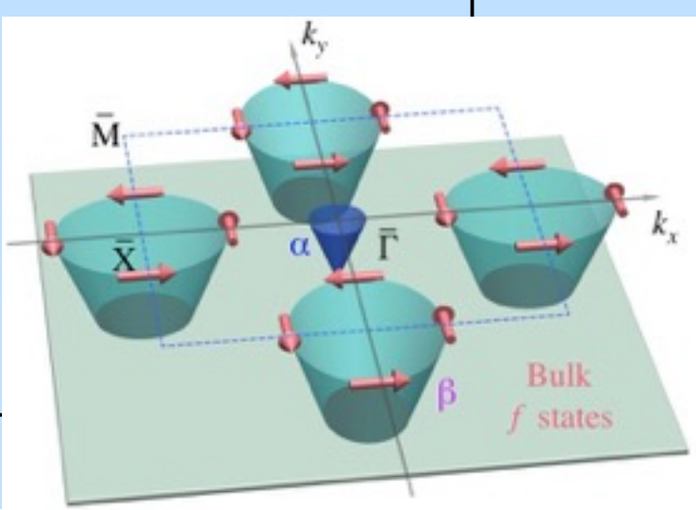
PAUL SCHERRER INSTITUT PSI

SWISS LIGHT SOURCE SLS

EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Swiss-Sino workshop, 4-6 May, 2015

(S-)ARPES investigation on the first topological Kondo insulator: SmB_6



Nan Xu

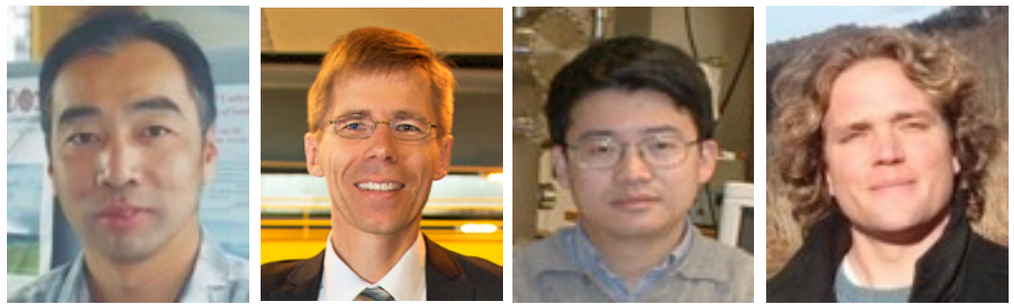
Swiss Light Source, Paul Scherrer Institut

& École polytechnique fédérale de Lausanne

Acknowledgment

(S-)ARPES measurements

PSI: **M. Shi, J. Mesot,** C. Matt, R. Dhaka, Y. Huang, N. Plumb, M. Radovic
IOP: **H. Ding,** X. Shi
COPHEE: **J. H. Dil**, G. Landolt, S. Muff
IFW: S.V. Borisenko

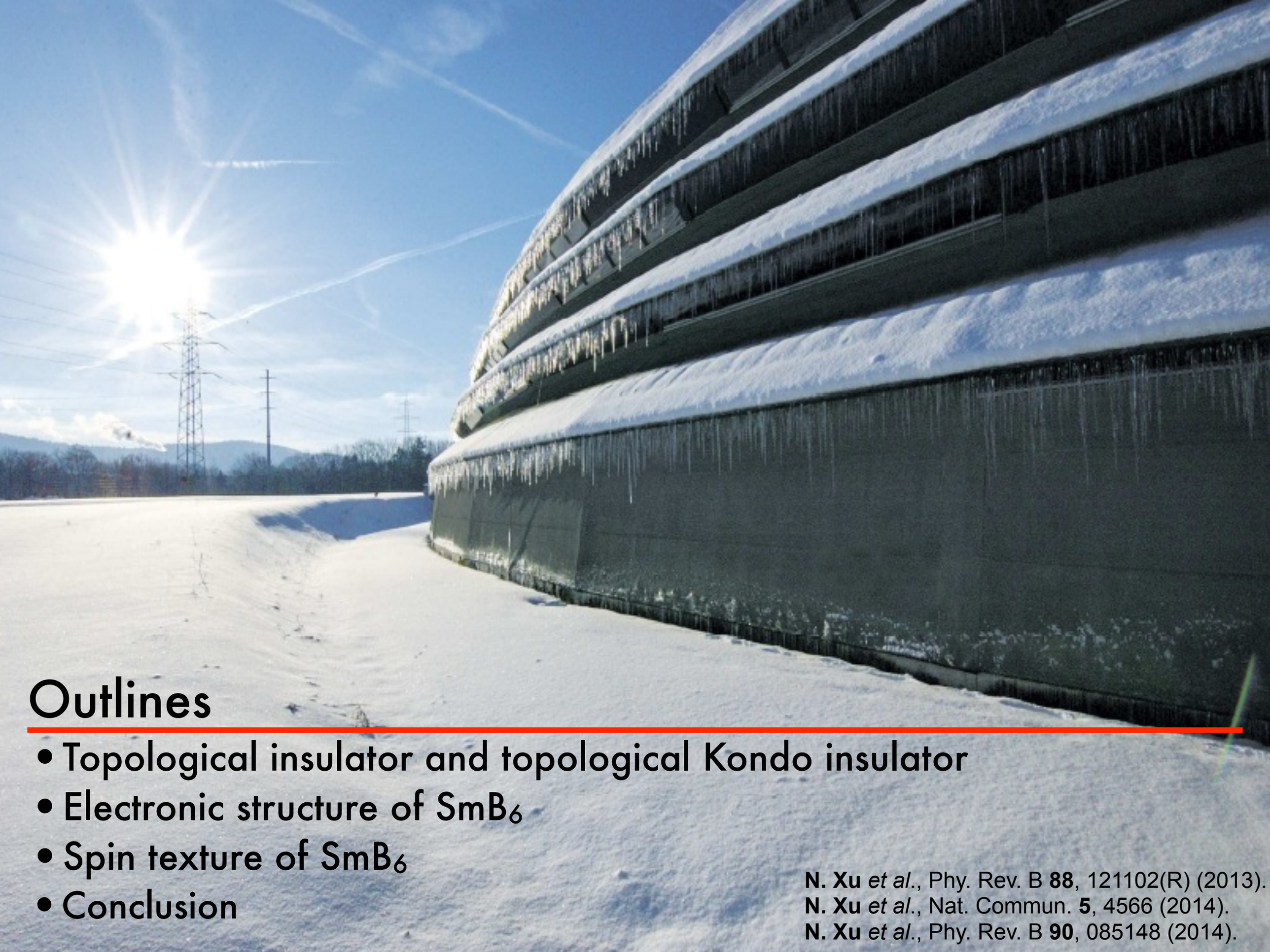


High-quality single crystals

PSI: **E. Pomjakushina**,K. Conder, P. Biswas, A. Amato, Z. Salman
University of Warwick: D. Paul

Theoretical support

IOP: **Z. Fang, X. Dai,** H. M. Weng, R. Yu

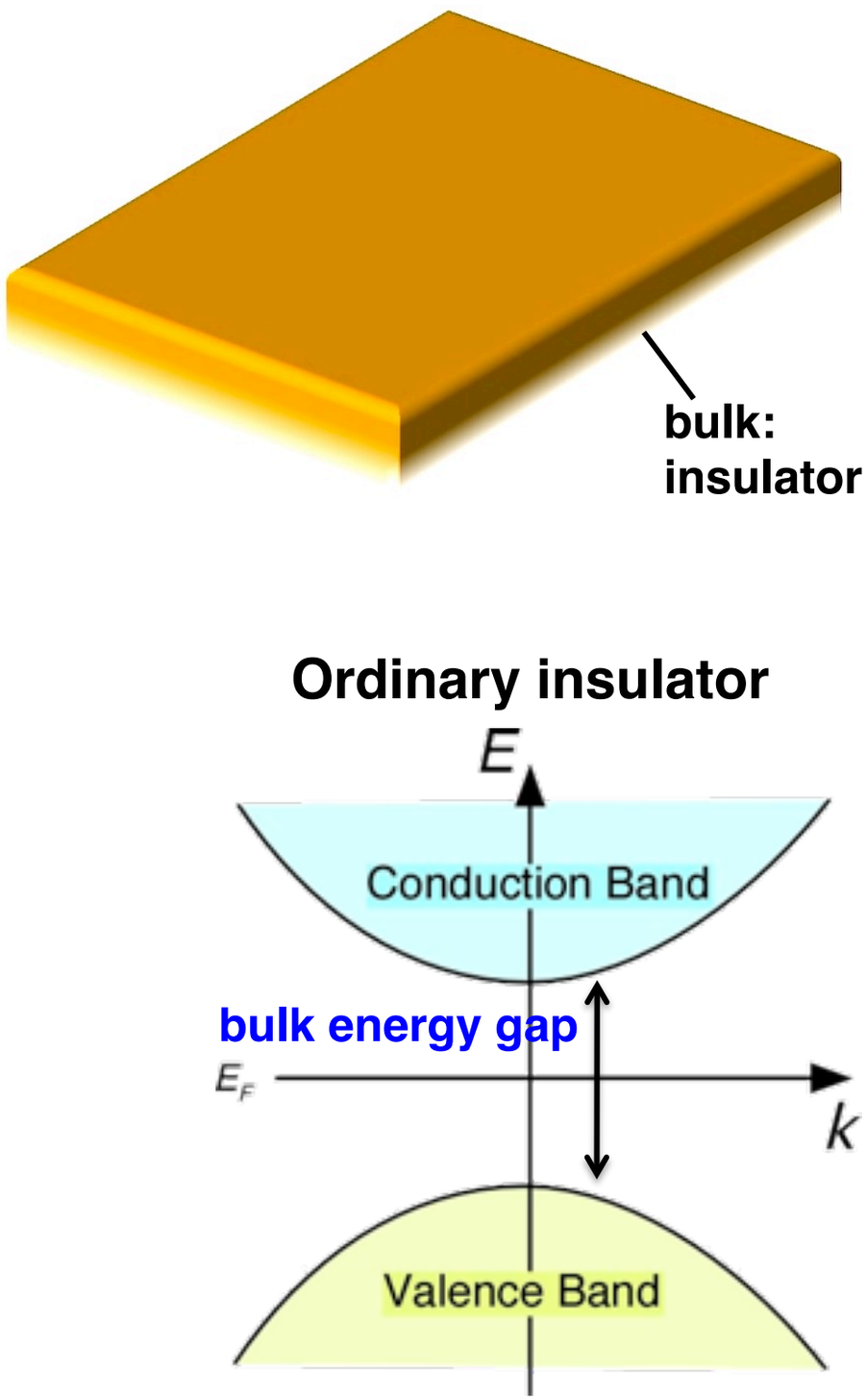


Outlines

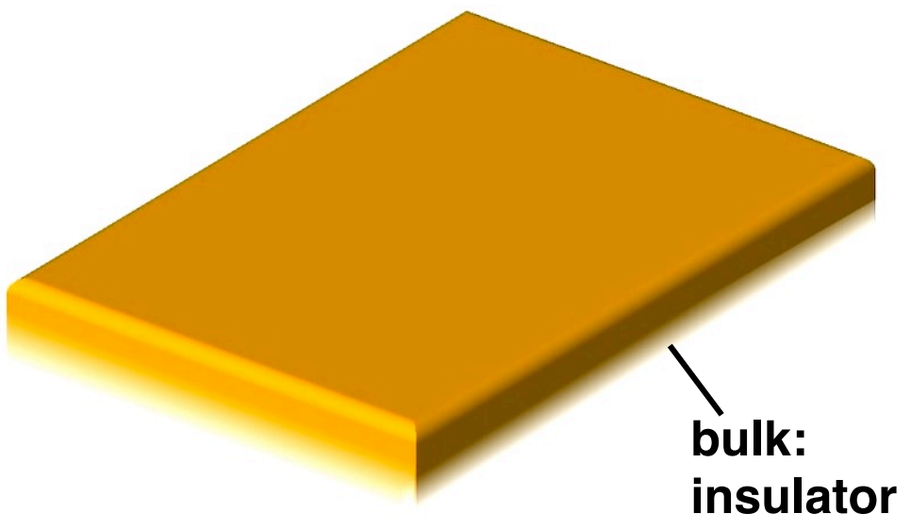
- Topological insulator and topological Kondo insulator
- Electronic structure of SmB_6
- Spin texture of SmB_6
- Conclusion

N. Xu *et al*., Phy. Rev. B **88**, 121102(R) (2013).
N. Xu *et al*., Nat. Commun. **5**, 4566 (2014).
N. Xu *et al*., Phy. Rev. B **90**, 085148 (2014).

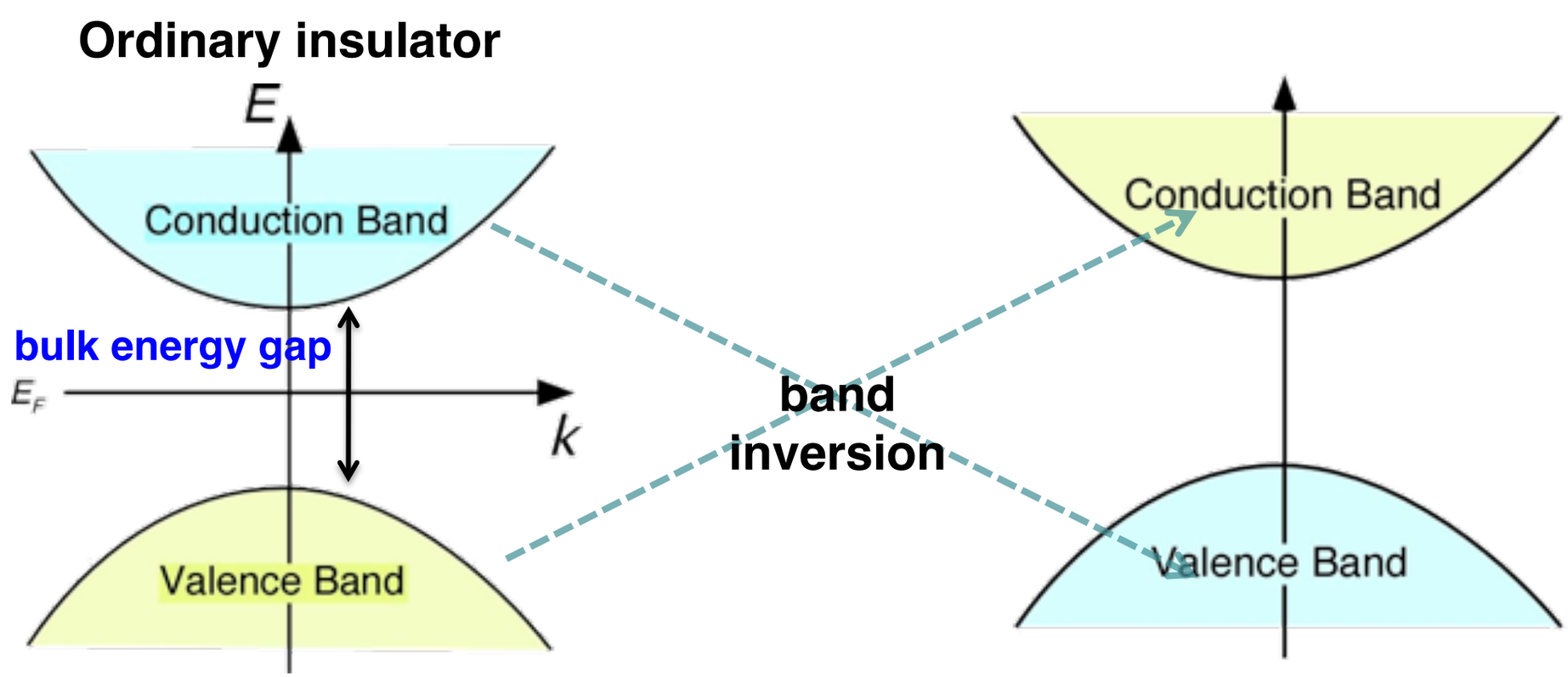
Topological Insulator



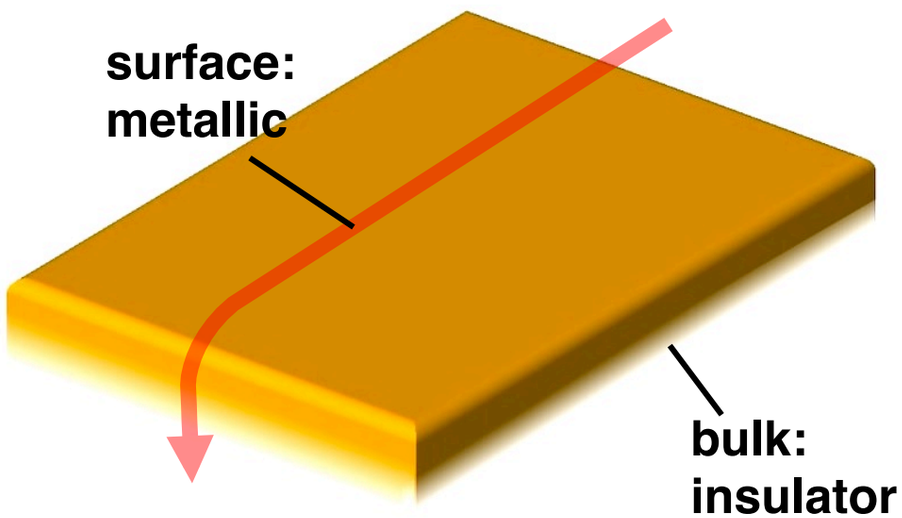
Topological Insulator



Spin-orbit interaction

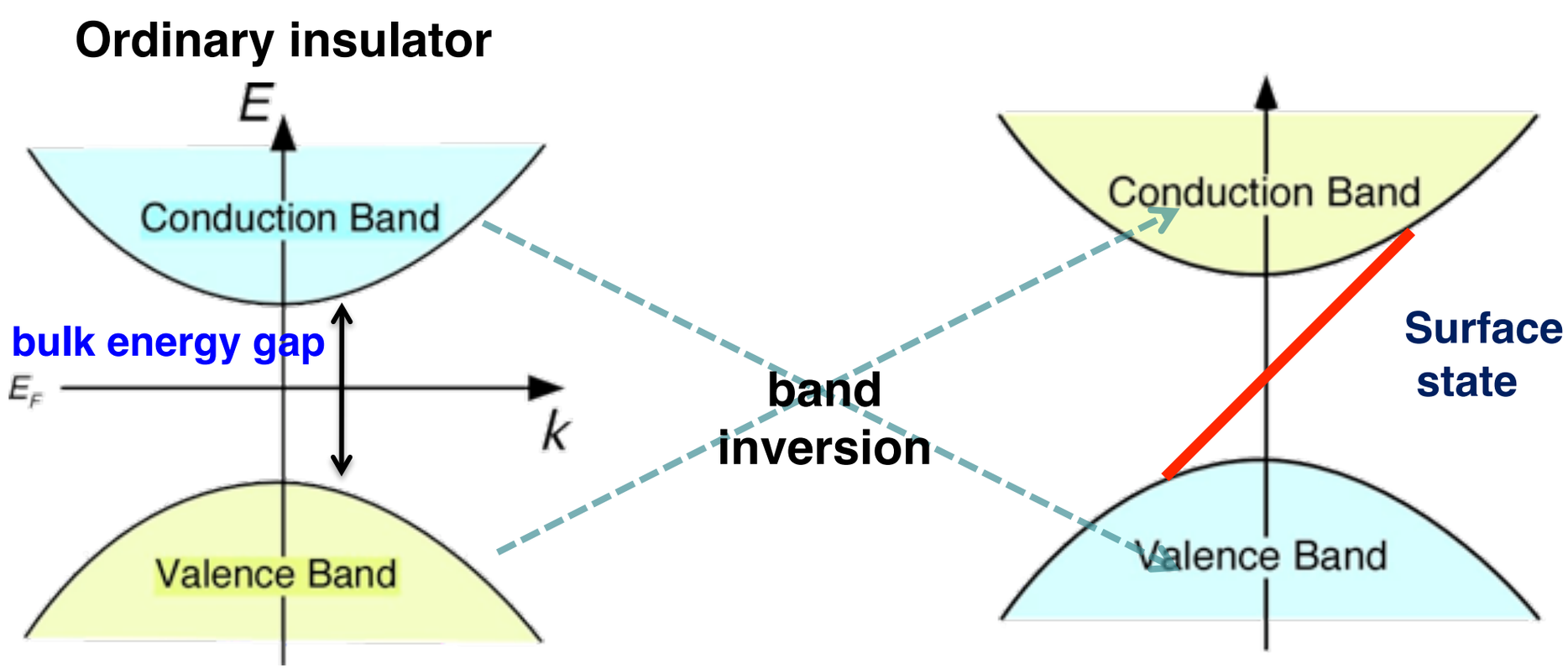


Topological Insulator

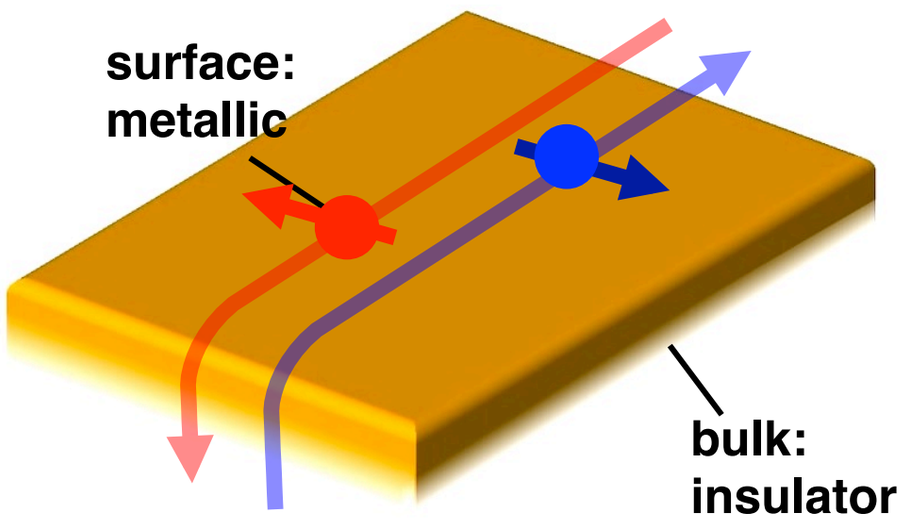


Spin-orbit interaction

+ Topology (surface)



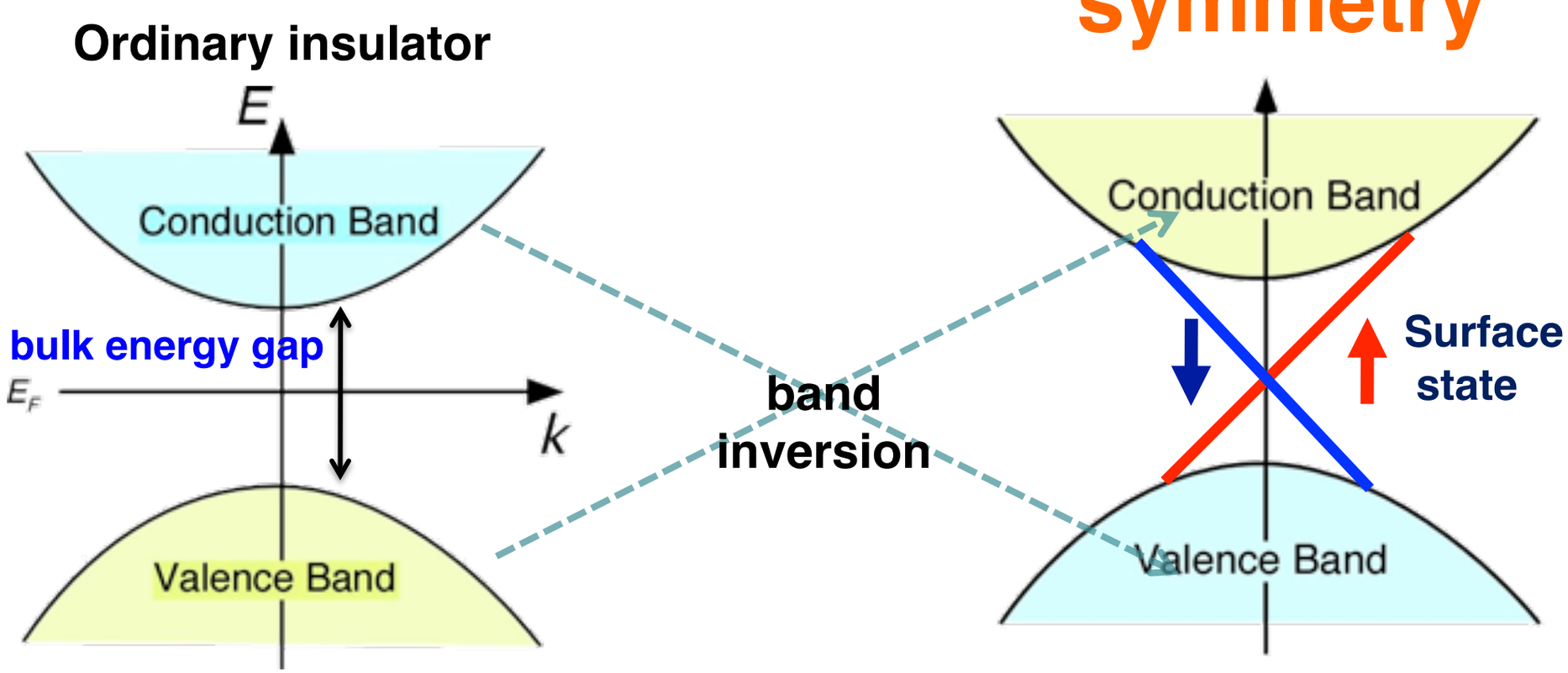
Topological Insulator



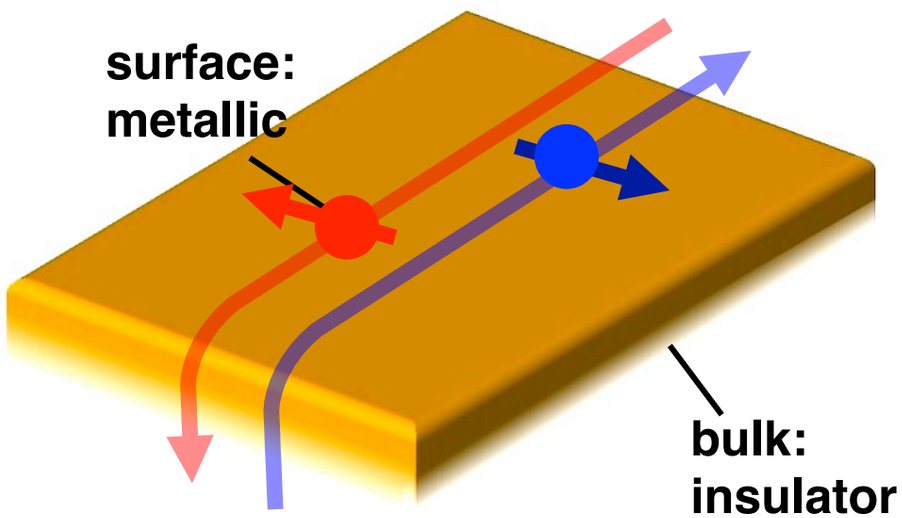
Spin-orbit interaction

+ Topology (surface)

+ Time reversal symmetry



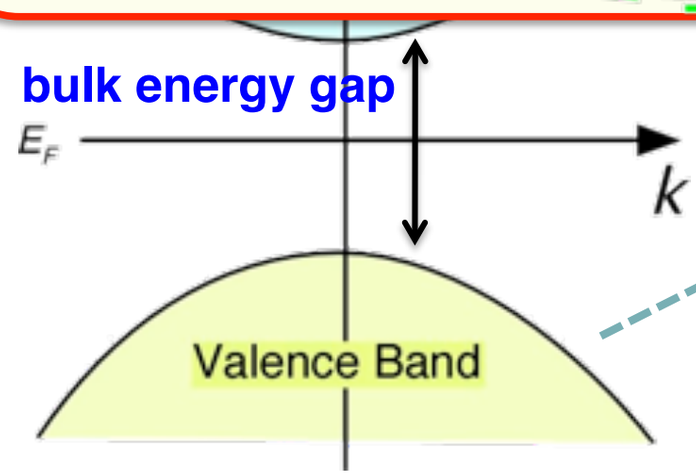
Topological Insulator



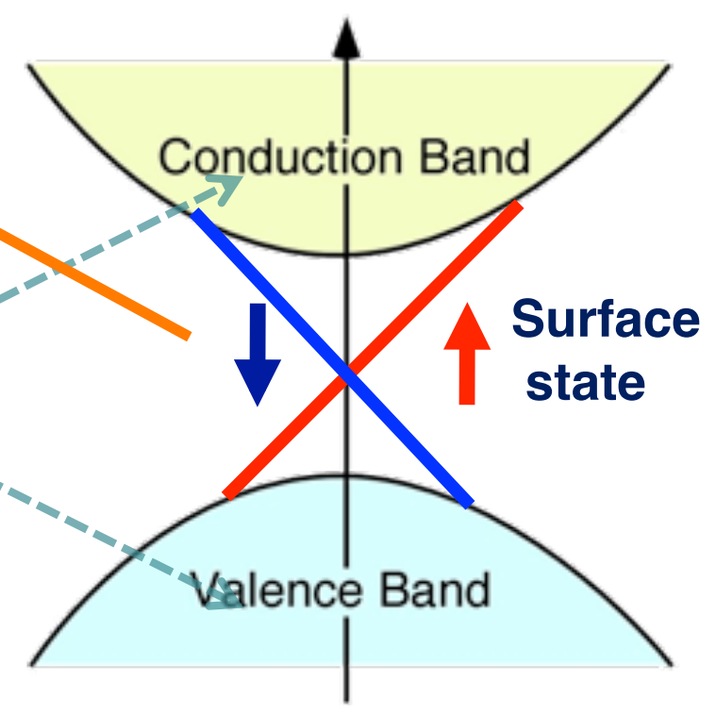
Spin-orbit interaction

+ Topology (surface)

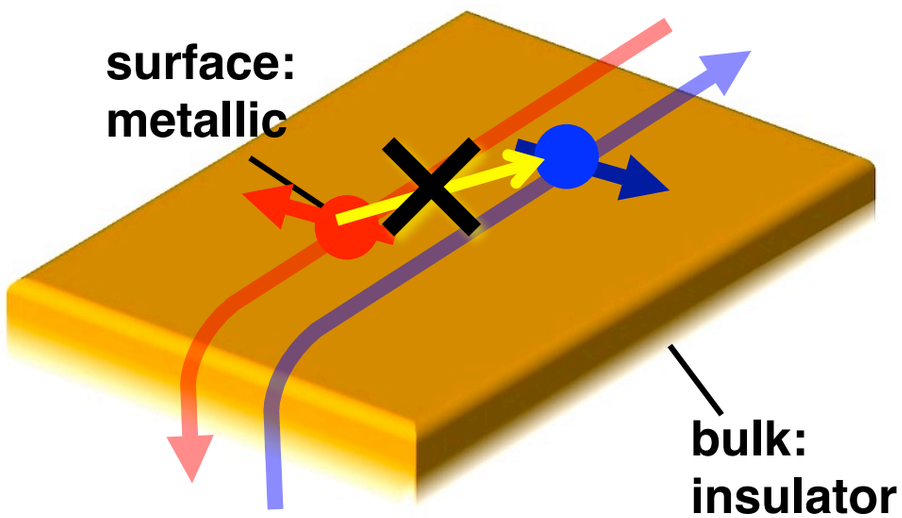
+ Time reversal symmetry



band
inversion



Topological Insulator



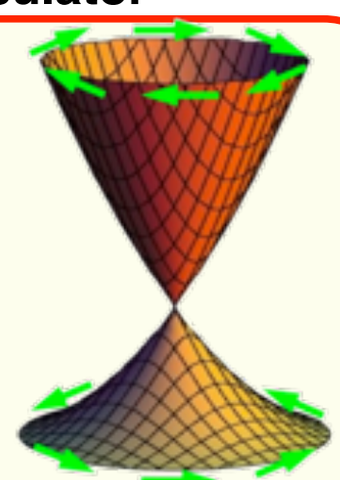
Spin-orbit interaction

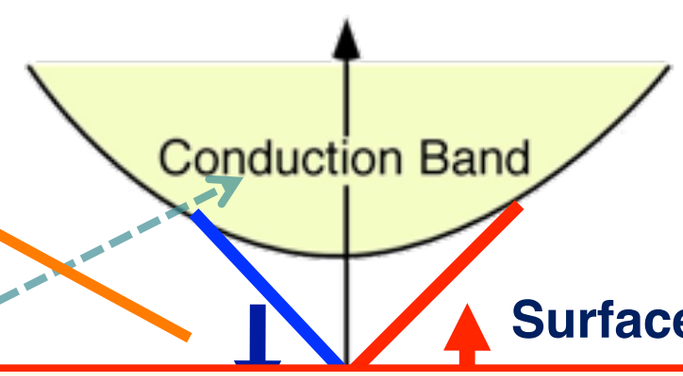
+ Topology (surface)

+ Time reversal symmetry

Dirac-cone state

helical spin





bulk energy gap

Characteristics of Dirac cone

- **Tunable spin-polarization by *E*-field**
- **Back-scattering prohibited : error-free devices**

No Bulk Insulating

Experimental

Table I. Summary of topological insulator materials that have bee experimentally addressed. The definiti table, S.S., P.T., and SM stand for surface state, phase transition, and semimetal, respectively.)

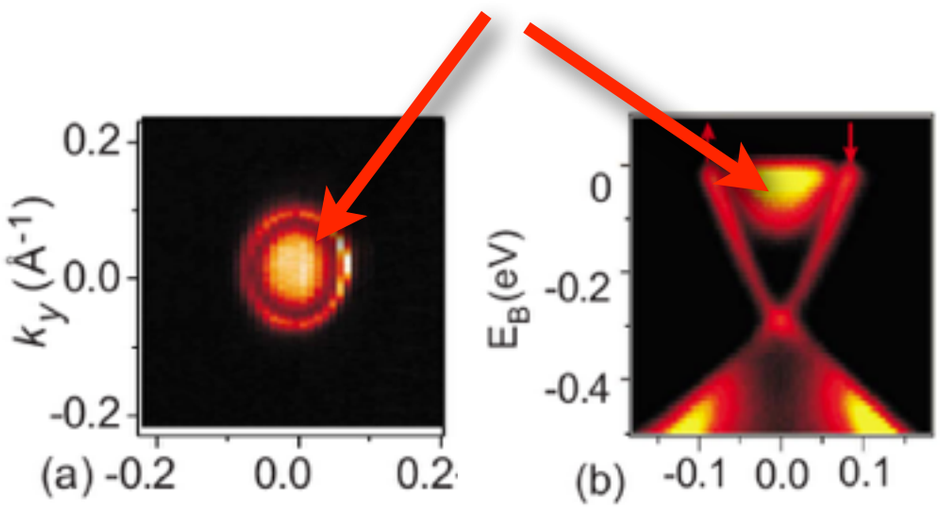
Type	Material	Band gap	Bulk transport
2D, $\nu = 1$	CdTe/HgTe/CdTe	< 10 meV	insulating
2D, $\nu = 1$	AlSb/InAs/GaSb/AlSb	~4 meV	weakly insulating
3D (1;111)	$Bi_{1-x}Sb_x$	< 30 meV	weakly insulating
3D (1;111)	Sb	semimetal	metallic
3D (1;000)	Bi_2Se_3	0.3 eV	metallic
3D (1;000)	Bi_2Te_3	0.17 eV	metallic
3D (1;000)	Sb_2Te_3	0.3 eV	metallic
3D (1;000)	Bi_2Te_2Se	~0.2 eV	reasonably insulating
3D (1;000)	$(Bi,Sb)_2Te_3$	< 0.2 eV	moderately insulating
3D (1;000)	$Bi_{2-x}Sb_xTe_{3-y}Se_y$	< 0.3 eV	reasonably insulating
3D (1;000)	$Bi_2Te_{1.6}S_{1.4}$	0.2 eV	metallic
3D (1;000)	$Bi_{1.1}Sb_{0.9}Te_2S$	0.2 eV	moderately insulating
3D (1;000)	Sb_2Te_2Se	?	metallic
3D (1;000)	$Bi_2(Te,Se)_2(Se,S)$	0.3 eV	semi-metallic
3D (1;000)	$TlBiSe_2$	~0.35 eV	metallic
3D (1;000)	$TlBiTe_2$	~0.2 eV	metallic
3D (1;000)	$TlBi(S,Se)_2$	< 0.35 eV	metallic
3D (1;000)	$PbBi_2Te_4$	~0.2 eV	metallic
3D (1;000)	$PbSb_2Te_4$	?	metallic
3D (1;000)	$GeBi_2Te_4$	0.18 eV	metallic
3D (1;000)	$PbBi_4Te_7$	0.2 eV	metallic
3D (1;000)	$GeBi_{4-x}Sb_xTe_7$	0.1–0.2 eV	metallic
3D (1;000)	$(PbSe)_5(Bi_2Se_3)_6$	0.5 eV	metallic
3D (1;000)	$(Bi_2)(Bi_2Se_{2.6}S_{0.4})$	semimetal	metallic
3D (1;000)	$(Bi_2)(Bi_2Te_3)_2$	?	?
3D TCI	SnTe	0.3 eV (4.2 K)	metallic
3D TCI	$Pb_{1-x}Sn_xTe$	< 0.3 eV	metallic
3D TCI	$Pb_{0.77}Sn_{0.23}Se$	invert with T	metallic
2D, $\nu = 1$?	Bi bilayer	~0.1 eV	?
3D (1;000)?	Ag_2Te	?	metallic
3D (1;111)?	SmB_6	20 meV	insulating
3D (0;001)?	$Bi_{14}Rh_3I_9$	0.27 eV	metallic
3D (1;000)?	RBiPt (R = Lu, Dy, Gd)	zero gap	metallic
Weyl SM?	$Nd_2(Ir_{1-x}Rh_x)_2O_7$	zero gap	metallic

Yoichi Ando, J. Phys. Soc. Jpn. 82, 102001 (2013)

No Bulk Insulating

Experimental

Bulk Conducting Band



D. Hsieh, *et al*., Nature, 460, 1101. (2009)

Table I. Summary of topological insulator materials that have bee experimentally addressed. The definiti table, S.S., P.T., and SM stand for surface state, phase transition, and semimetal, respectively.)

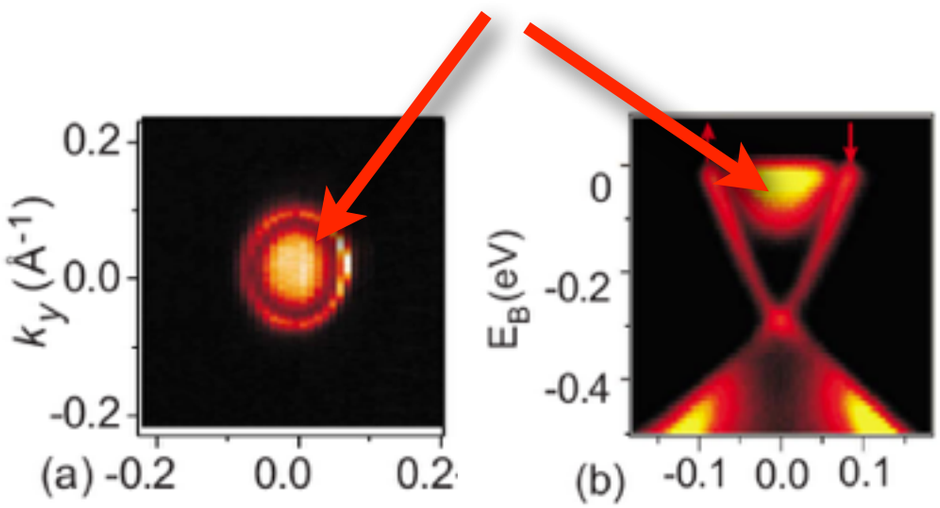
Type	Material	Band gap	Bulk transport
2D, $\nu = 1$	CdTe/HgTe/CdTe	< 10 meV	insulating
2D, $\nu = 1$	AlSb/InAs/GaSb/AlSb	~4 meV	weakly insulating
3D (1;111)	$Bi_{1-x}Sb_x$	< 30 meV	weakly insulating
3D (1;111)	Sb	semimetal	metallic
3D (1;000)	Bi_2Se_3	0.3 eV	metallic
3D (1;000)	Bi_2Te_3	0.17 eV	metallic
3D (1;000)	Sb_2Te_3	0.3 eV	metallic
3D (1;000)	Bi_2Te_2Se	~0.2 eV	reasonably insulating
3D (1;000)	$(Bi,Sb)_2Te_3$	< 0.2 eV	moderately insulating
3D (1;000)	$Bi_{2-x}Sb_xTe_{3-y}Se_y$	< 0.3 eV	reasonably insulating
3D (1;000)	$Bi_2Te_{1.6}S_{1.4}$	0.2 eV	metallic
3D (1;000)	$Bi_{1.1}Sb_{0.9}Te_2S$	0.2 eV	moderately insulating
3D (1;000)	Sb_2Te_2Se	?	metallic
3D (1;000)	$Bi_2(Te,Se)_2(Se,S)$	0.3 eV	semi-metallic
3D (1;000)	$TlBiSe_2$	~0.35 eV	metallic
3D (1;000)	$TlBiTe_2$	~0.2 eV	metallic
3D (1;000)	$TlBi(S,Se)_2$	< 0.35 eV	metallic
3D (1;000)	$PbBi_2Te_4$	~0.2 eV	metallic
3D (1;000)	$PbSb_2Te_4$	?	metallic
3D (1;000)	$GeBi_2Te_4$	0.18 eV	metallic
3D (1;000)	$PbBi_4Te_7$	0.2 eV	metallic
3D (1;000)	$GeBi_{4-x}Sb_xTe_7$	0.1–0.2 eV	metallic
3D (1;000)	$(PbSe)_5(Bi_2Se_3)_6$	0.5 eV	metallic
3D (1;000)	$(Bi_2)(Bi_2Se_{2.6}S_{0.4})$	semimetal	metallic
3D (1;000)	$(Bi_2)(Bi_2Te_3)_2$	?	?
3D TCI	SnTe	0.3 eV (4.2 K)	metallic
3D TCI	$Pb_{1-x}Sn_xTe$	< 0.3 eV	metallic
3D TCI	$Pb_{0.77}Sn_{0.23}Se$	invert with T	metallic
2D, $\nu = 1$?	Bi bilayer	~0.1 eV	?
3D (1;000)?	Ag_2Te	?	metallic
3D (1;111)?	SmB_6	20 meV	insulating
3D (0;001)?	$Bi_{14}Rh_3I_9$	0.27 eV	metallic
3D (1;000)?	RBiPt (R = Lu, Dy, Gd)	zero gap	metallic
Weyl SM?	$Nd_2(Ir_{1-x}Rh_x)_2O_7$	zero gap	metallic

Yoichi Ando, J. Phys. Soc. Jpn. 82, 102001 (2013)

No Bulk Insulating

Experimental

Bulk Conducting Band



D. Hsieh, *et al*., Nature, 460, 1101. (2009)

No Bulk insulating

- Transport measurements
- Bulk sensitive measurements
- Spintronics applications

Table I. Summary of topological insulator materials that have bee experimentally addressed. The definiti table, S.S., P.T., and SM stand for surface state, phase transition, and semimetal, respectively.)

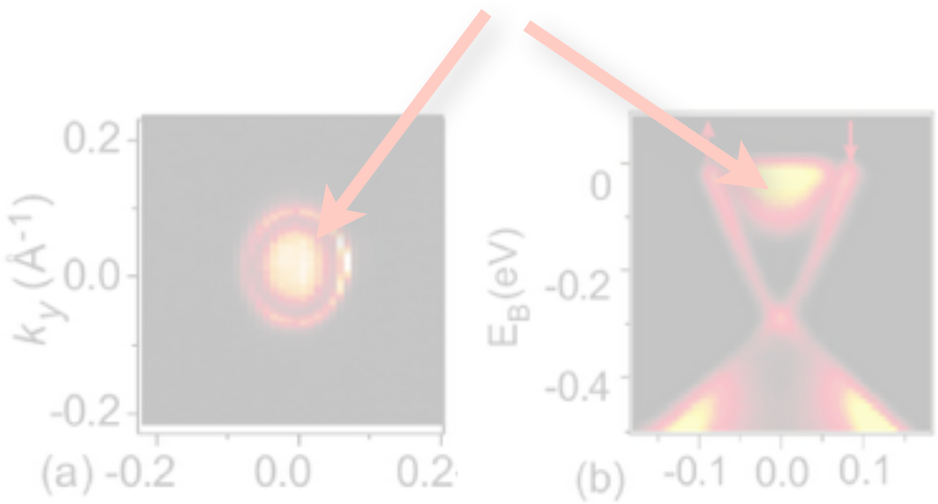
Type	Material	Band gap	Bulk transport
2D, $\nu = 1$	CdTe/HgTe/CdTe	< 10 meV	insulating
2D, $\nu = 1$	AlSb/InAs/GaSb/AlSb	~4 meV	weakly insulating
3D (1;111)	$Bi_{1-x}Sb_x$	< 30 meV	weakly insulating
3D (1;111)	Sb	semimetal	metallic
3D (1;000)	Bi_2Se_3	0.3 eV	metallic
3D (1;000)	Bi_2Te_3	0.17 eV	metallic
3D (1;000)	Sb_2Te_3	0.3 eV	metallic
3D (1;000)	Bi_2Te_2Se	~0.2 eV	reasonably insulating
3D (1;000)	$(Bi,Sb)_2Te_3$	< 0.2 eV	moderately insulating
3D (1;000)	$Bi_{2-x}Sb_xTe_{3-y}Se_y$	< 0.3 eV	reasonably insulating
3D (1;000)	$Bi_2Te_{1.6}S_{1.4}$	0.2 eV	metallic
3D (1;000)	$Bi_{1.1}Sb_{0.9}Te_2S$	0.2 eV	moderately insulating
3D (1;000)	Sb_2Te_2Se	?	metallic
3D (1;000)	$Bi_2(Te,Se)_2(Se,S)$	0.3 eV	semi-metallic
3D (1;000)	$TlBiSe_2$	~0.35 eV	metallic
3D (1;000)	$TlBiTe_2$	~0.2 eV	metallic
3D (1;000)	$TlBi(S,Se)_2$	< 0.35 eV	metallic
3D (1;000)	$PbBi_2Te_4$	~0.2 eV	metallic
3D (1;000)	$PbSb_2Te_4$	?	metallic
3D (1;000)	$GeBi_2Te_4$	0.18 eV	metallic
3D (1;000)	$PbBi_4Te_7$	0.2 eV	metallic
3D (1;000)	$GeBi_{4-x}Sb_xTe_7$	0.1–0.2 eV	metallic
3D (1;000)	$(PbSe)_5(Bi_2Se_3)_6$	0.5 eV	metallic
3D (1;000)	$(Bi_2)(Bi_2Se_{2.6}S_{0.4})$	semimetal	metallic
3D (1;000)	$(Bi_2)(Bi_2Te_3)_2$	?	?
3D TCI	SnTe	0.3 eV (4.2 K)	metallic
3D TCI	$Pb_{1-x}Sn_xTe$	< 0.3 eV	metallic
3D TCI	$Pb_{0.77}Sn_{0.23}Se$	invert with T	metallic
2D, $\nu = 1$?	Bi bilayer	~0.1 eV	?
3D (1;000)?	Ag_2Te	?	metallic
3D (1;111)?	SmB_6	20 meV	insulating
3D (0;001)?	$Bi_{14}Rh_3I_9$	0.27 eV	metallic
3D (1;000)?	RBiPt (R = Lu, Dy, Gd)	zero gap	metallic
Weyl SM?	$Nd_2(Ir_{1-x}Rh_x)_2O_7$	zero gap	metallic

Yoichi Ando, J. Phys. Soc. Jpn. 82, 102001 (2013)

Correlation effect

Experimental

Bulk Conducting Band



No Bulk insulating

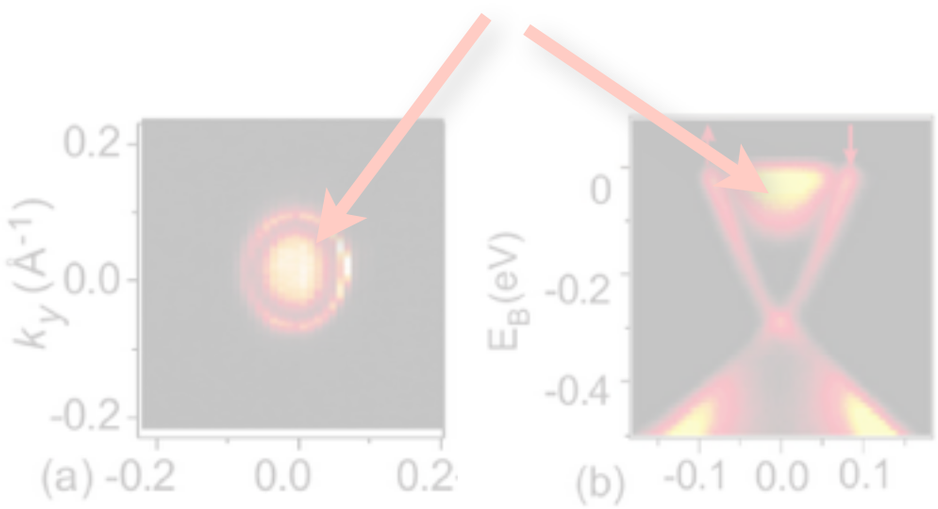
- Transport measurements
- Bulk sensitive measurements
- Spintronics applications

D. Hsieh, *et al*., Nature, 460, 1101. (2009)

Correlation effect

Experimental

Bulk Conducting Band



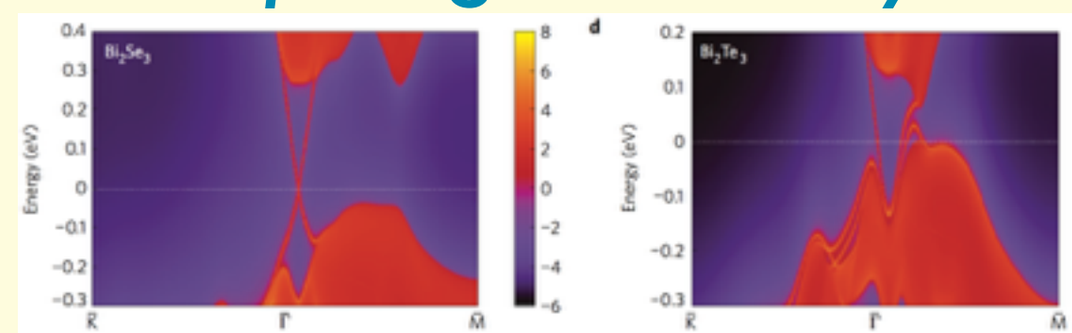
No Bulk insulating

- Transport measurements
- Bulk sensitive measurements
- Spintronics applications

D. Hsieh, *et al*., Nature, 460, 1101. (2009)

Theoretical

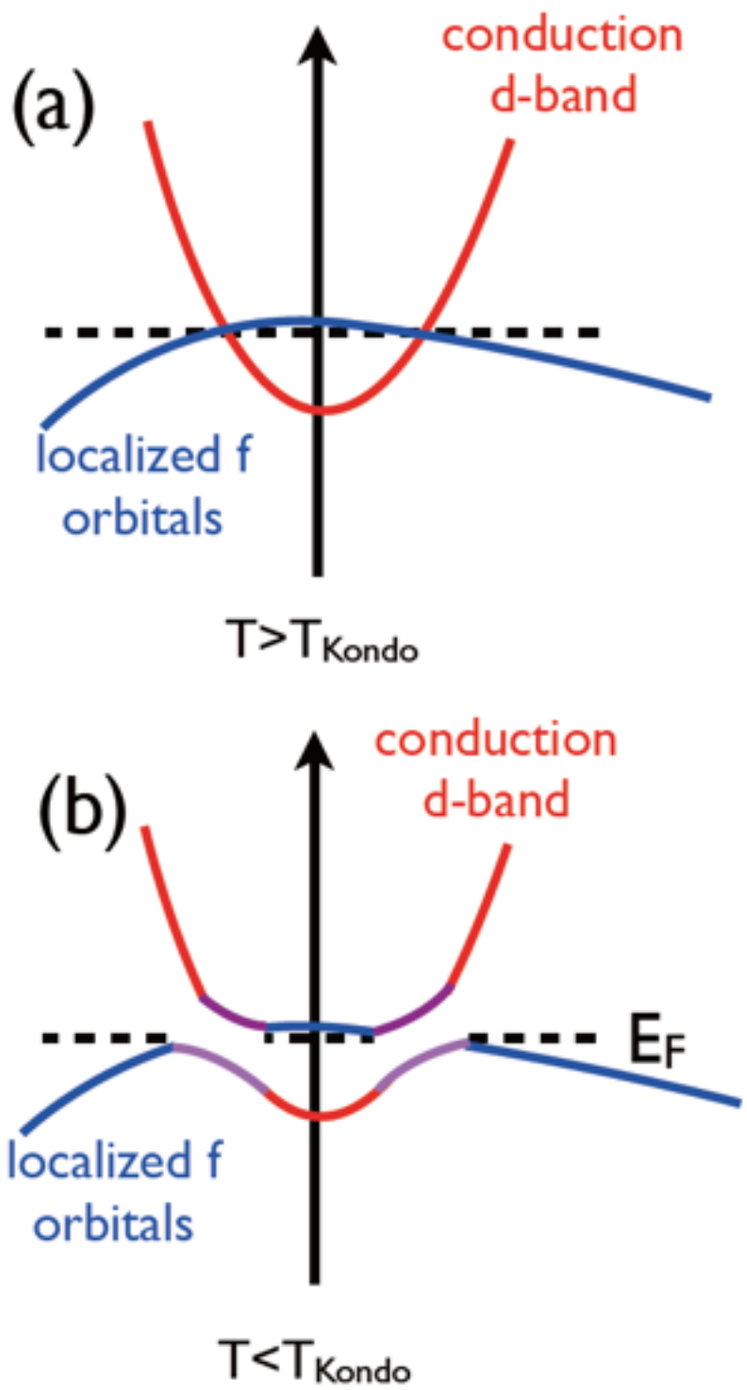
Non(weak)-interacting Topological theory



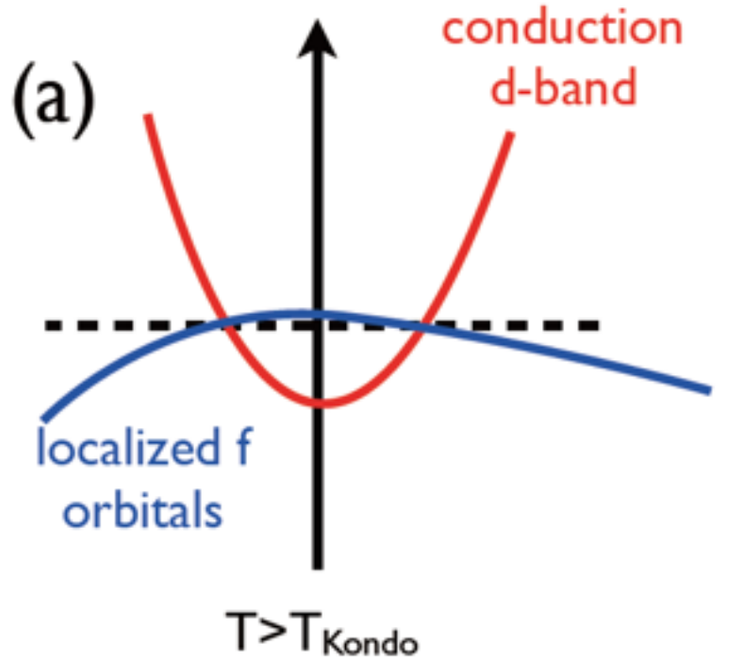
H. Zhang, *et al*., Nature Physics, 5, 438. (2009)
X.-L. Qi, S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
M.Z. Hasan, C.L. Kane, Rev. Mod. Phys.82, 3045(2010).

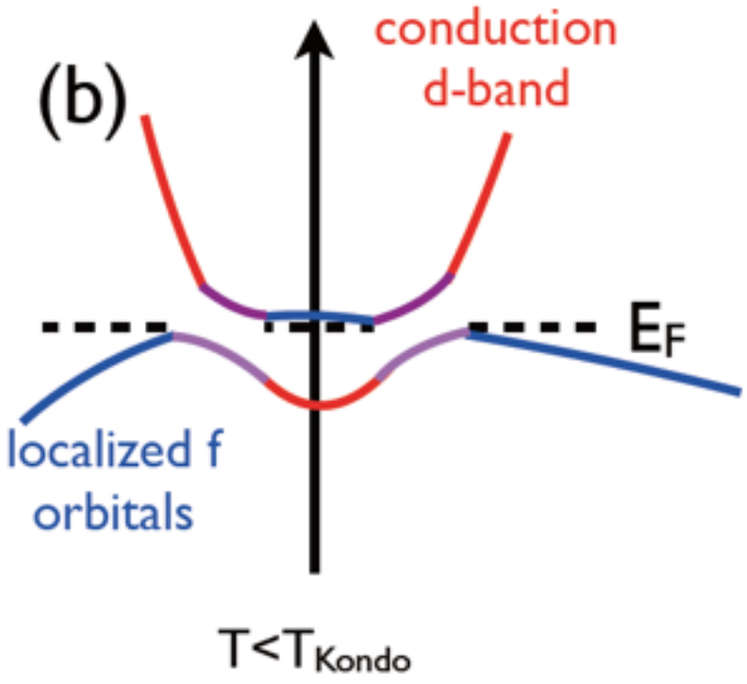
Weak e-e correlation

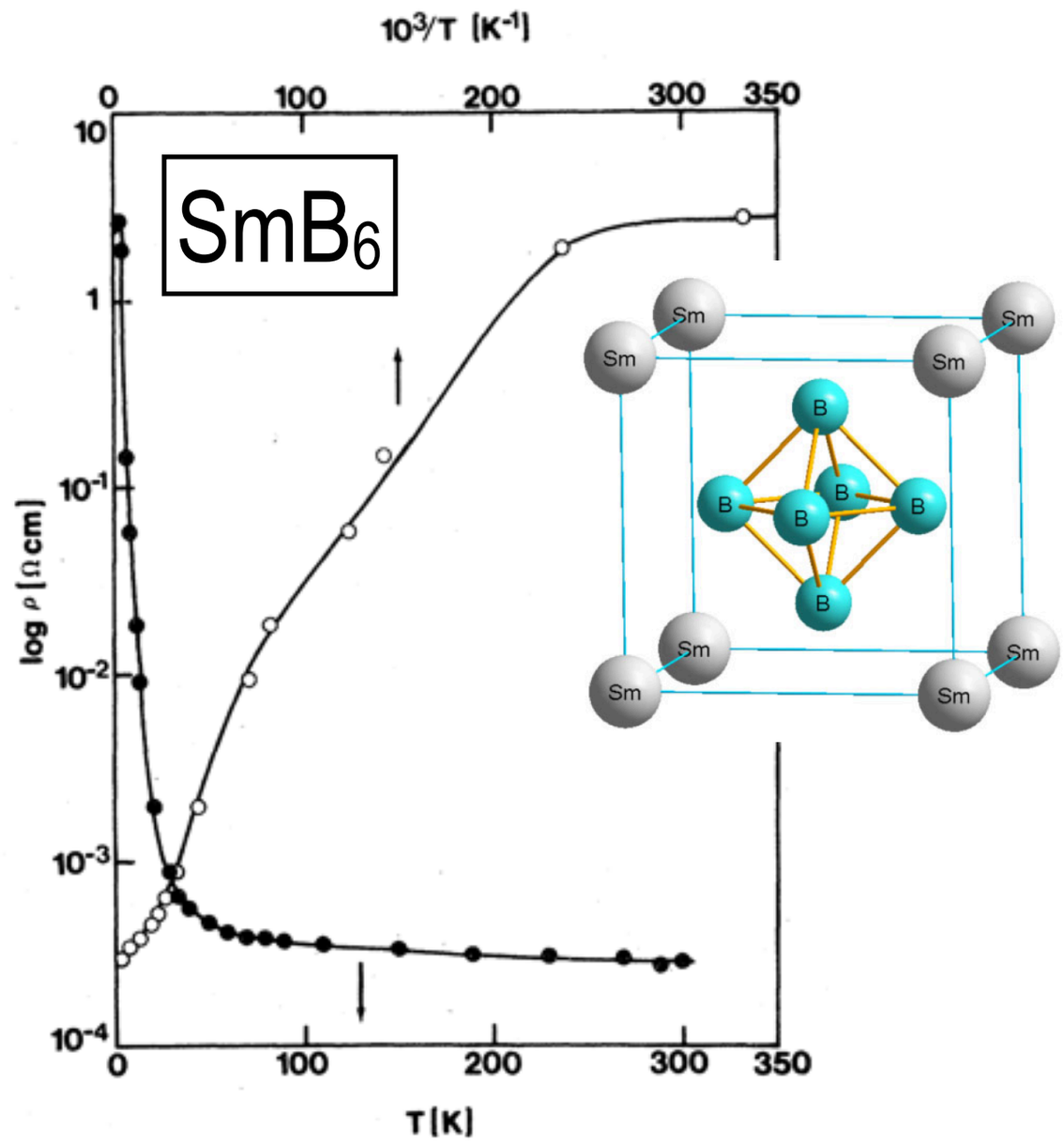
Kondo Insulator



Kondo Insulator





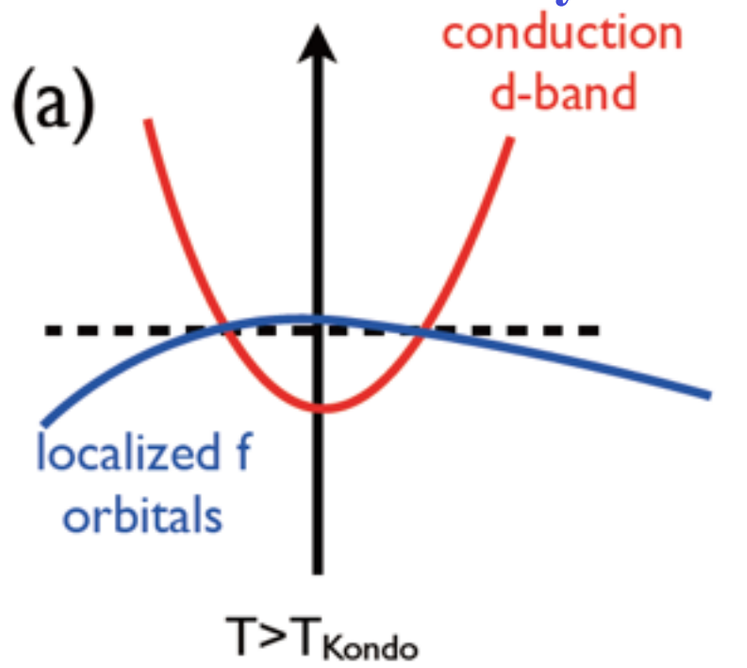


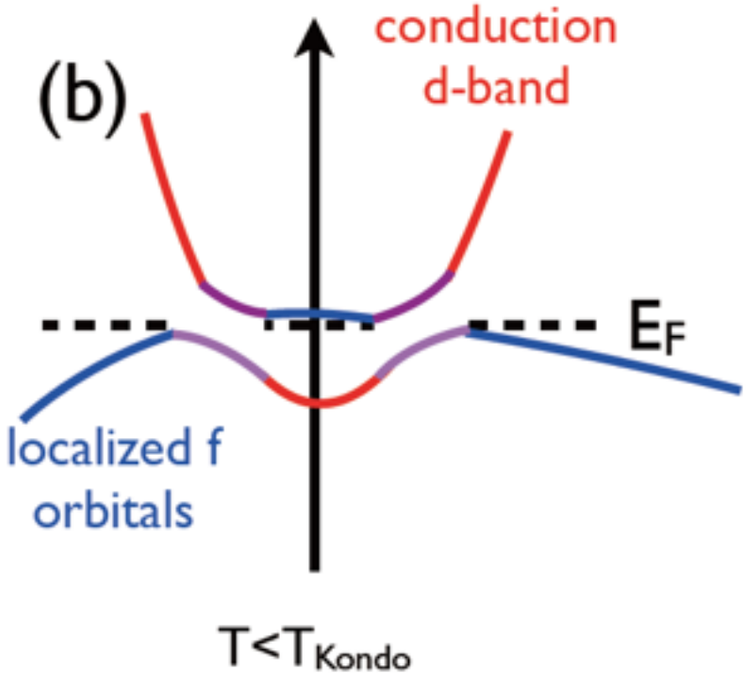
J. W. Allen, B. Batlogg, and P. Wachter, Phys. Rev. B. **20**, 4807 (1979).

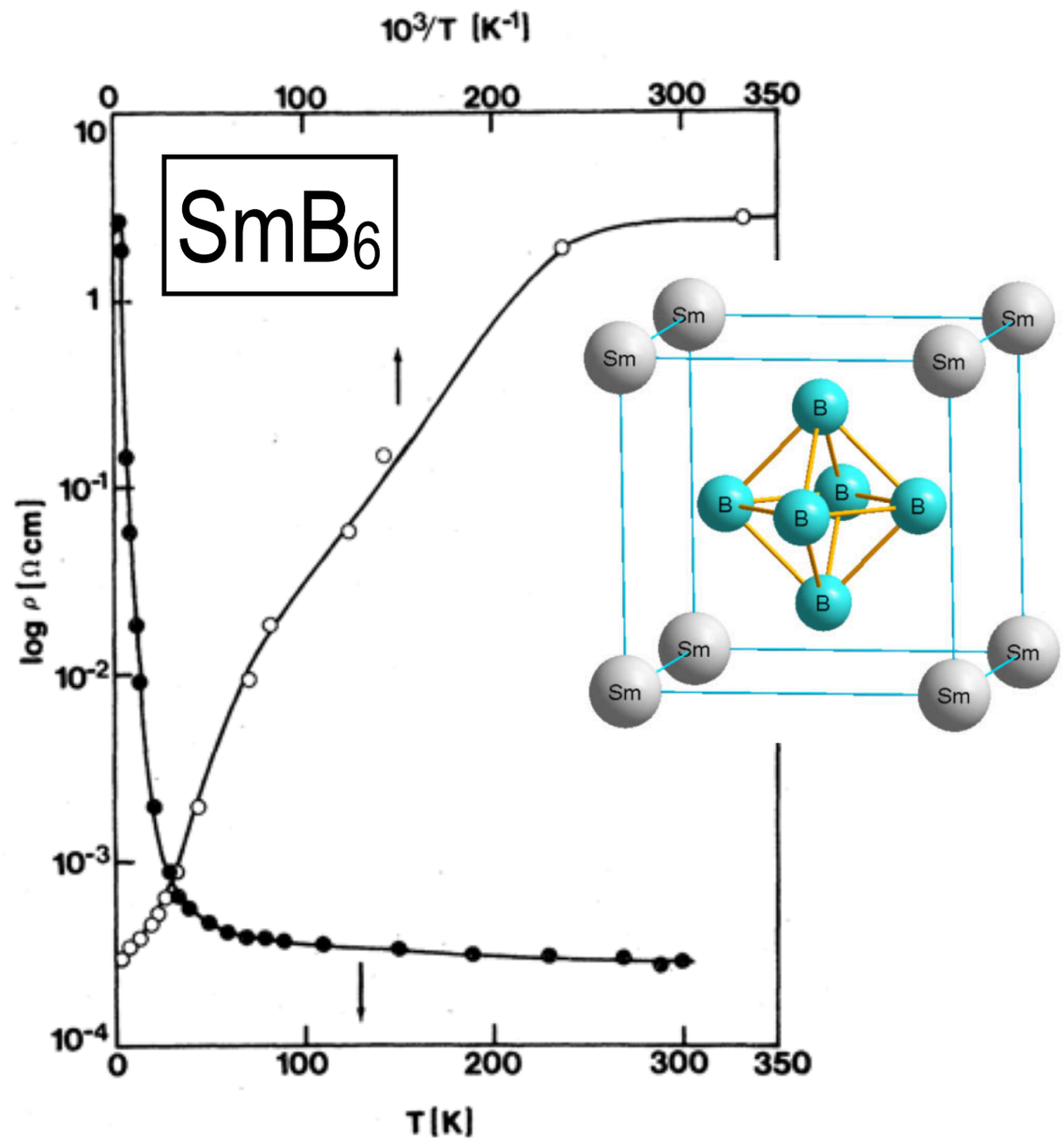
Topological Kondo Insulator

M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. **104**, 106408 (2010).
M. Dzero, K. Sun, P. Coleman and V. Galitski, Phys. Rev. B **85**, 045130 (2012).

Band-inversion naturally exists





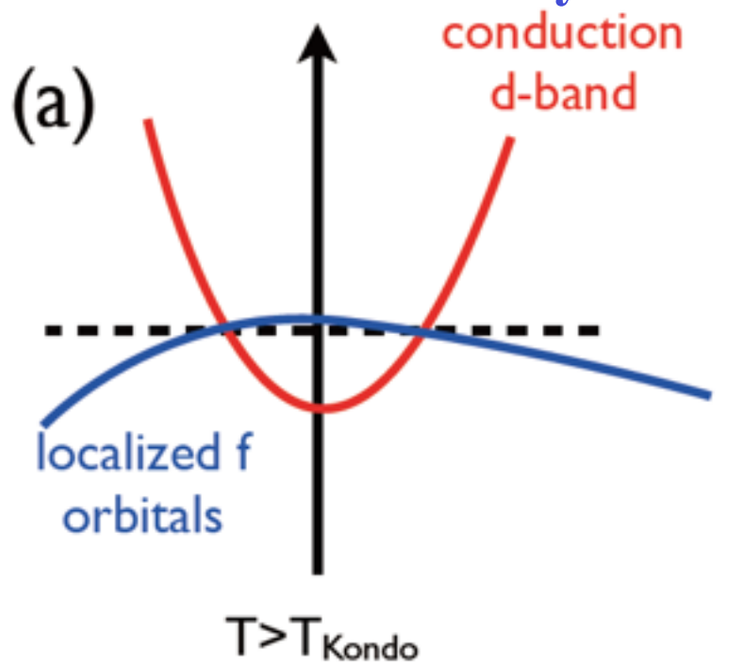


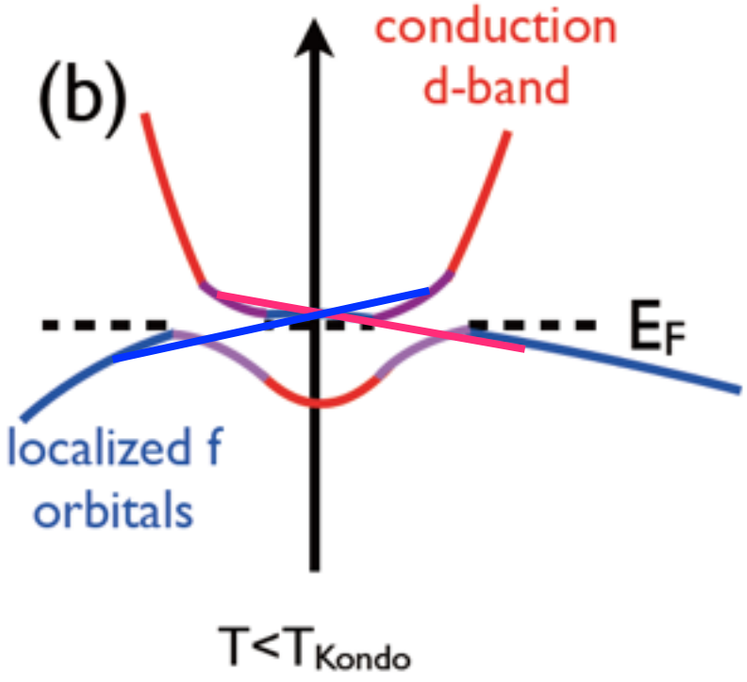
J. W. Allen, B. Batlogg, and P. Wachter, Phys. Rev. B. **20**, 4807 (1979).

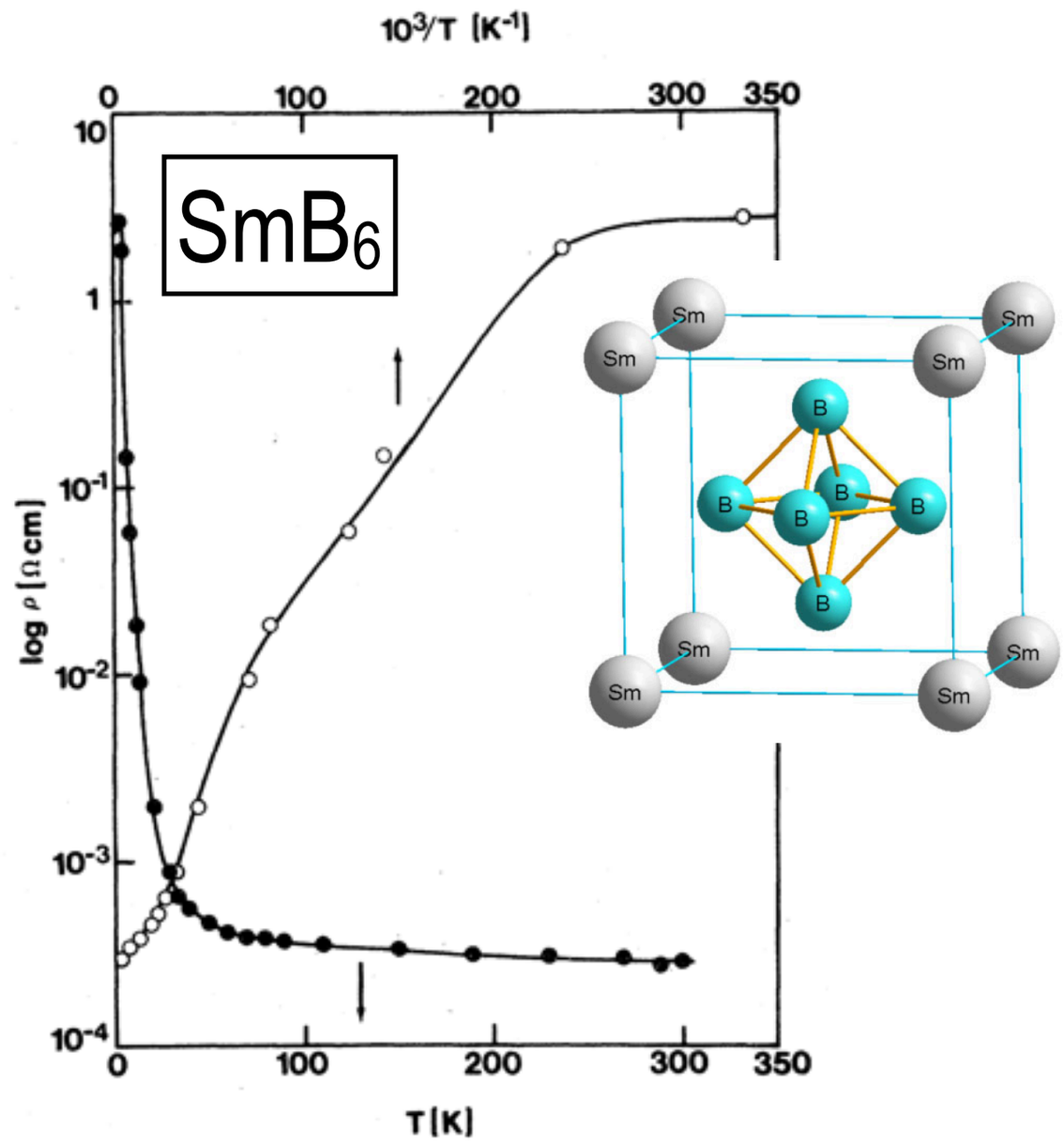
Topological Kondo Insulator

M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. **104**, 106408 (2010).
M. Dzero, K. Sun, P. Coleman and V. Galitski, Phys. Rev. B **85**, 045130 (2012).

Band-inversion naturally exists

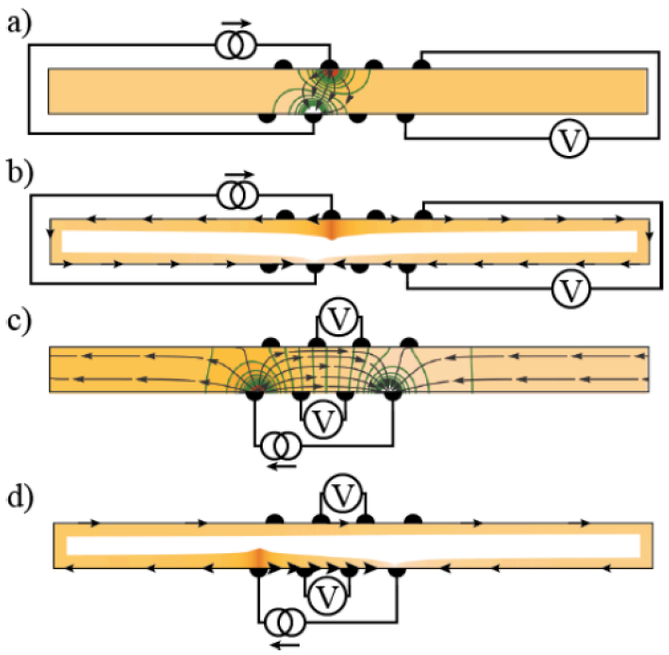


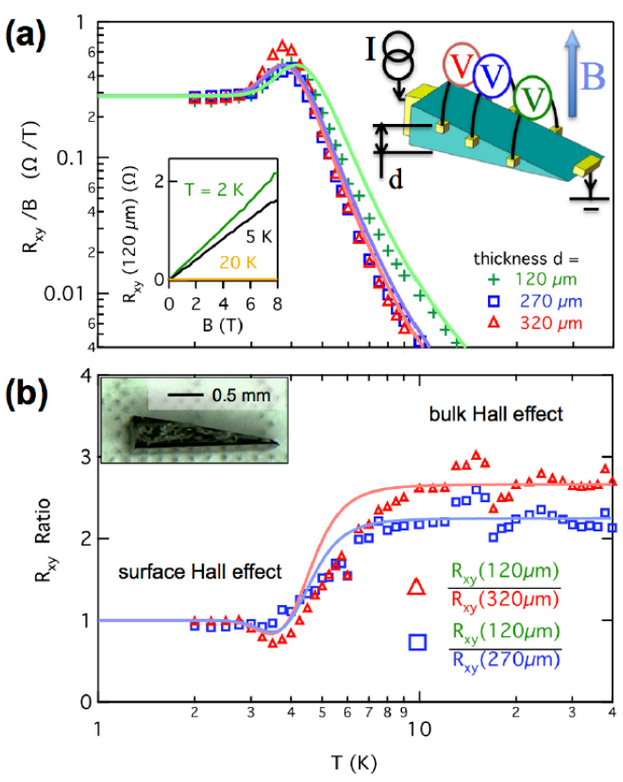


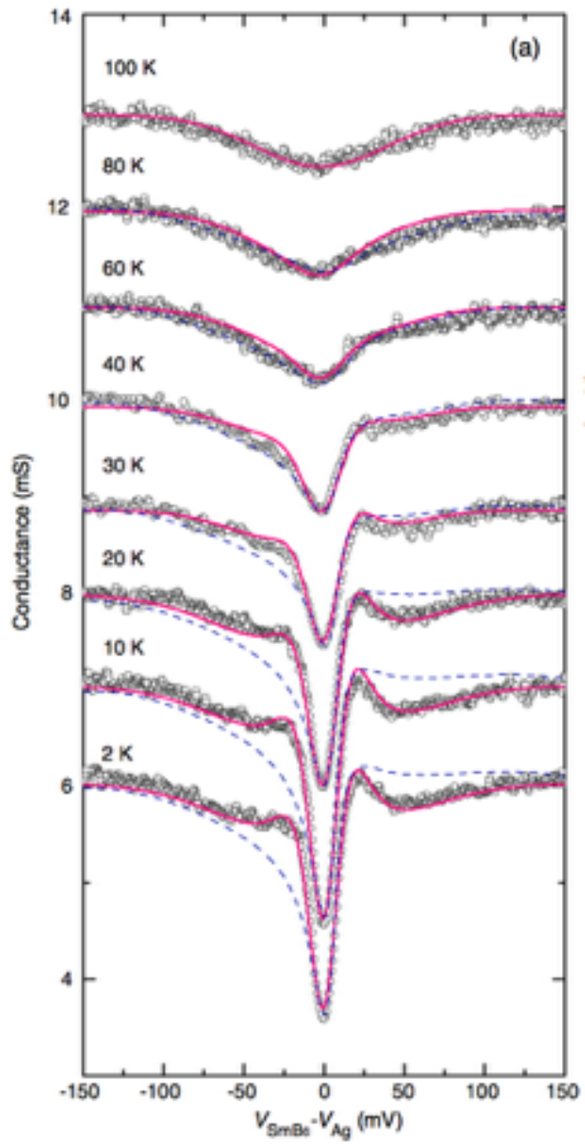


J. W. Allen, B. Batlogg, and P. Wachter, Phys. Rev. B. **20**, 4807 (1979).

Transport evidence of Robust SS







X. H. Zhang et al., Phys. Rev. X 3, 011011 (2013).

J. Botimer et al., arXiv, 1211.6769 (2012).

S. Wolgast et al., Phys. Rev. B 88, 180405 (2013).

D. Kim et al., Scientific Reports 3, 3150 (2013).

D. Kim, J. Xia and Z. Fisk, Nat. Mate. 13, 466 (2014)

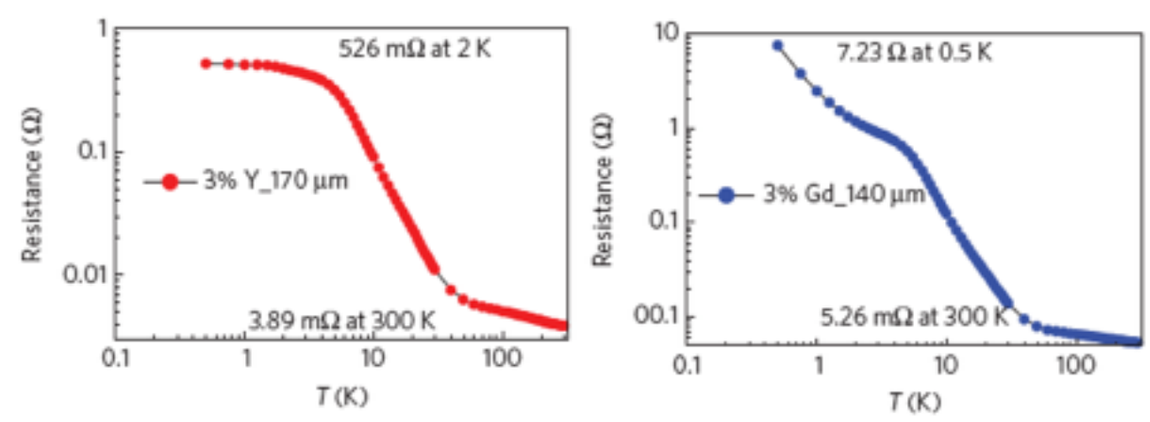
Thomas et al., arXiv.org (2013), 1307.4133.

G. Li et al., Science 346, 1208 (2014)

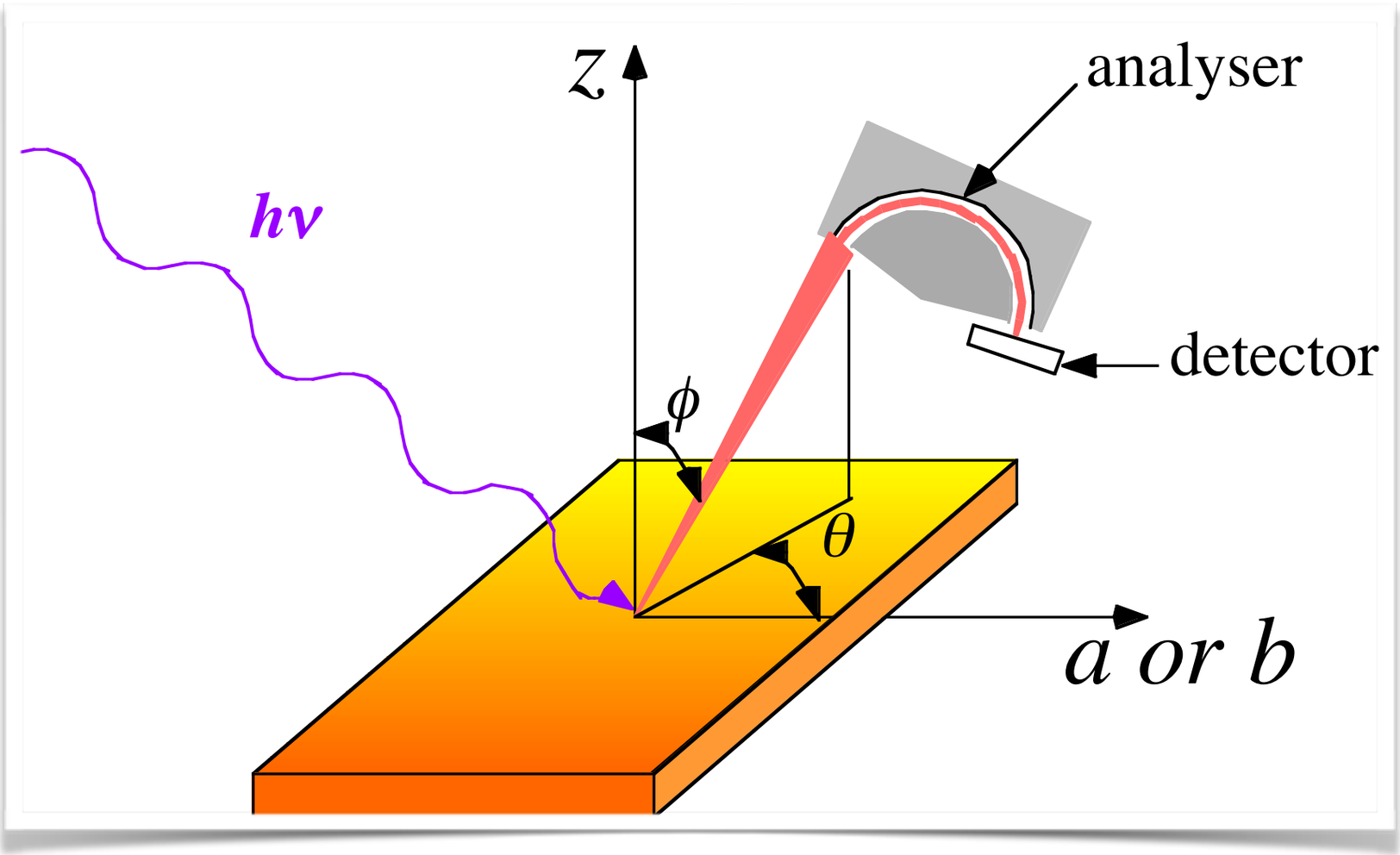
F. Chen et al. arXiv.org (2013), 1309.2378.

Z.-J. Yue et al., arXiv.org (2013), 1309.3005.

… …



Angle-Resolved Photo Emission Spectroscopy



Energy conservation

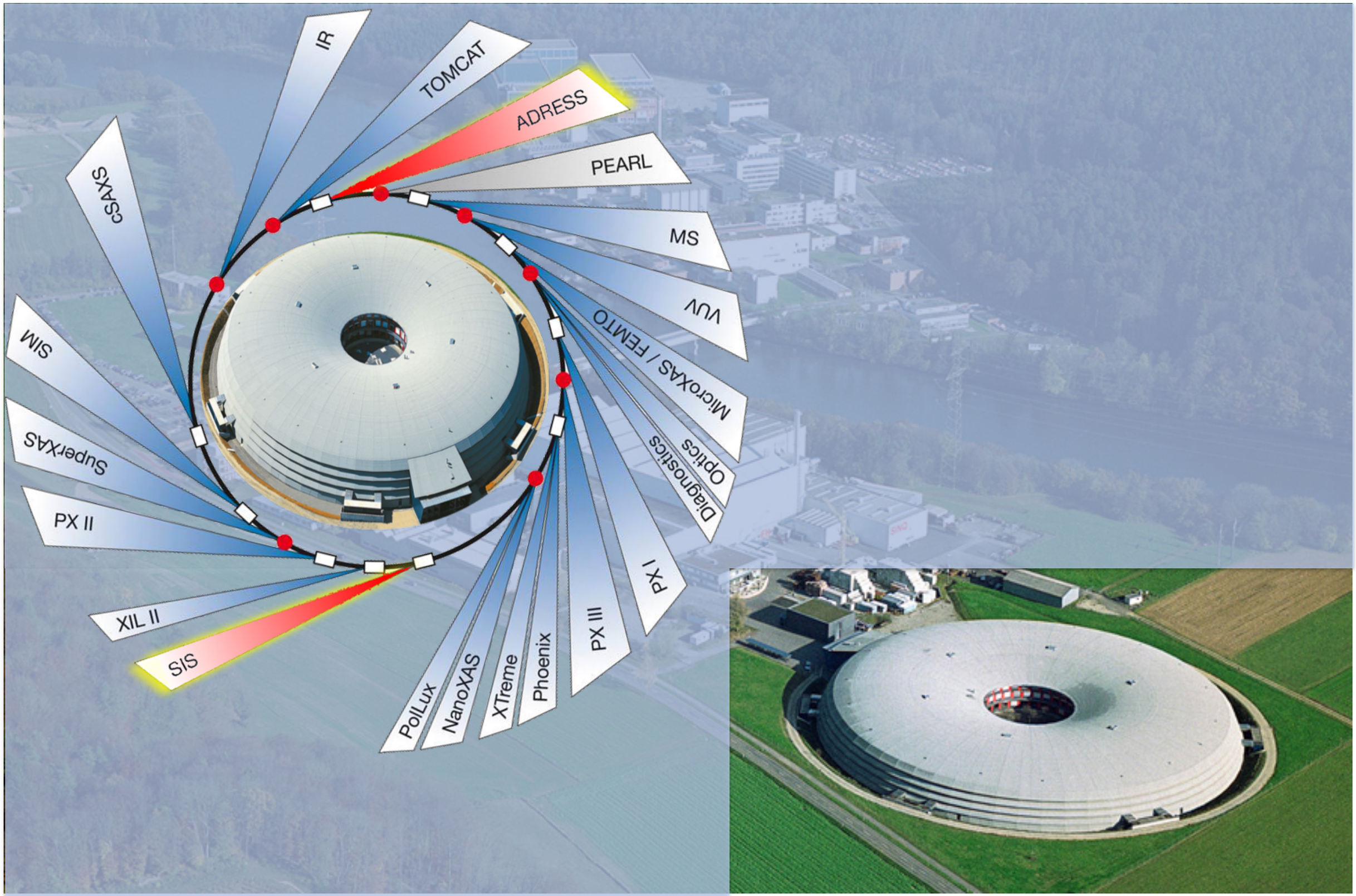
$$E_B = h\nu - E_k - \Phi$$

Momentum conservation

$$K_{||} = k_{||} + G_{||}$$

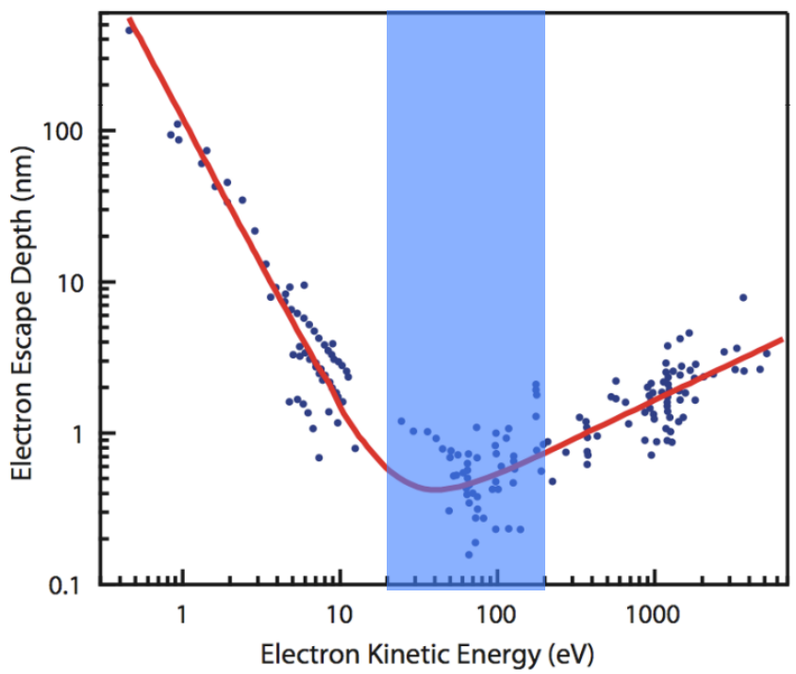
Swiss Light Source, PSI

Swiss Light Source, PSI



ARPES @ SLS

From M. P. Seah and W. A. Dench,
Surf. Interf. Anal. 1, 2 (1979).

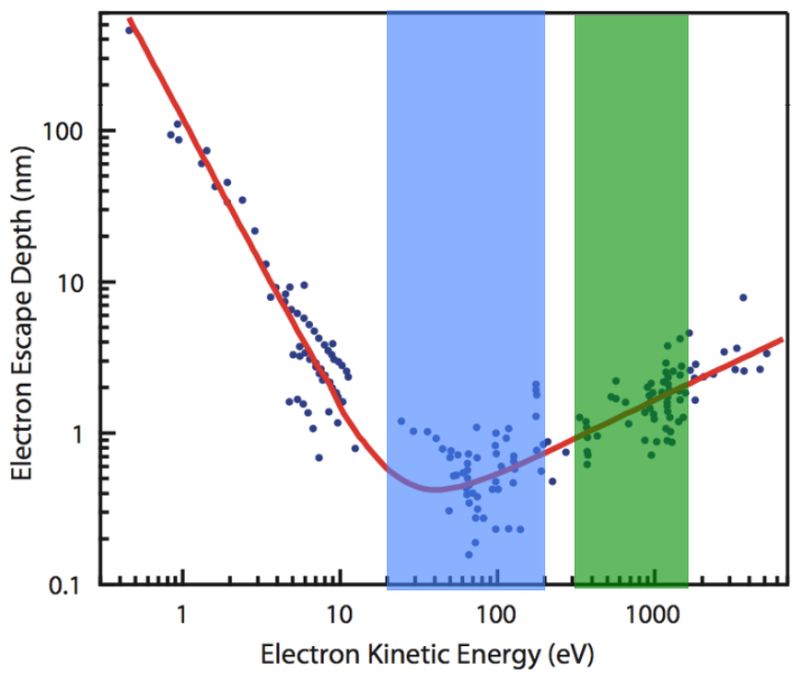


UV (HR)ARPES @ SIS beamline

Energy range: 10 – 800 eV
(optimized @ 20 – 200 eV)
Flux on sample: $2x10^{15}$ ph/s
0.1%BW @ 20 eV
Foot print: 50 x 100 μm^2
Resolution: < 5 meV @ 20 eV
Analyzer: VG-SCIENTA R4000

ARPES @ SLS

From M. P. Seah and W. A. Dench,
Surf. Interf. Anal. 1, 2 (1979).

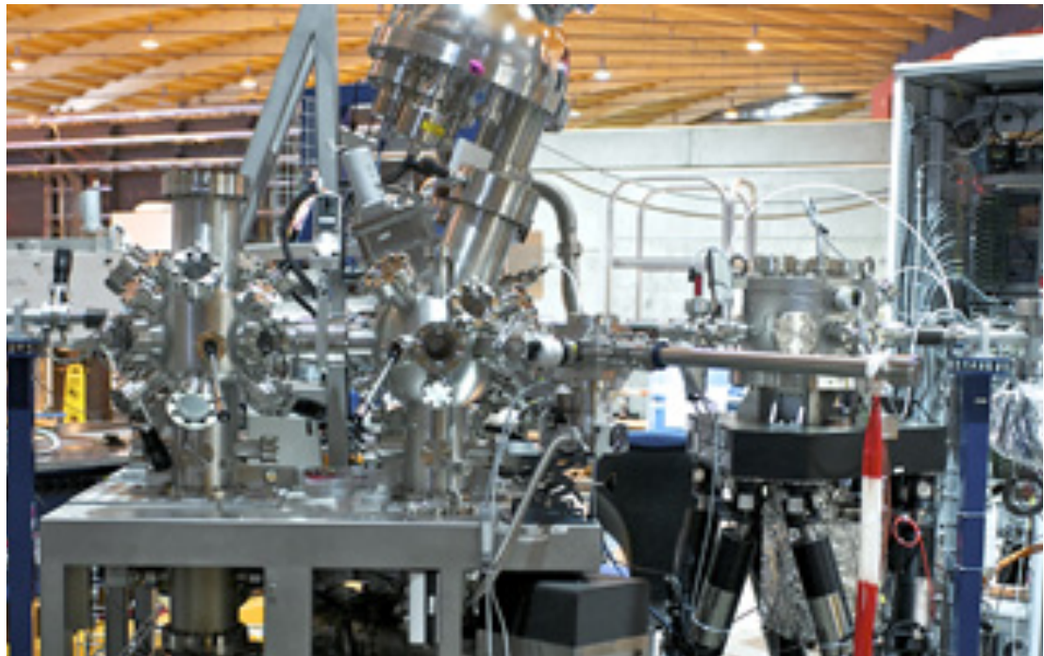


UV (HR)ARPES @ SIS beamline

Energy range: 10 – 800 eV
(optimized @ 20 – 200 eV)
Flux on sample: $2x10^{15}$ ph/s
0.1%BW @ 20 eV
Foot print: 50 x 100 μm^2
Resolution: < 5 meV @ 20 eV
Analyzer: VG-SCIENTA R4000

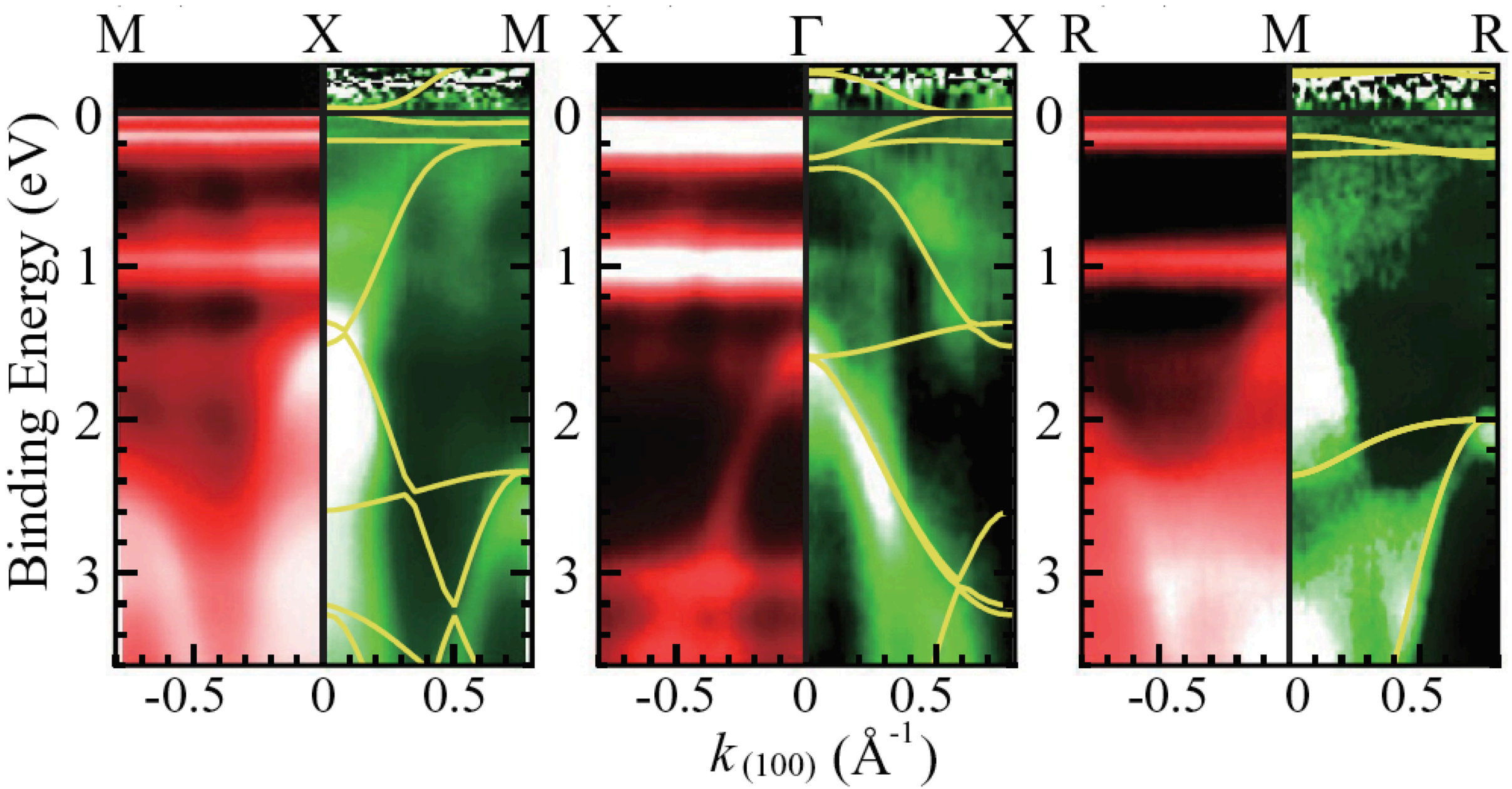
Soft-X-ray ARPES @ ADRESS beamline

Energy range: 300 – 1600 eV
Flux on sample: 10^{13}ph/s/0.01%BW @ 1keV
Spot size: 30 x 70 m^2
Resolution: 60 meV @ 1 keV (25~30 meV below 600 eV)
Analyzer: PHOIBIOS-150



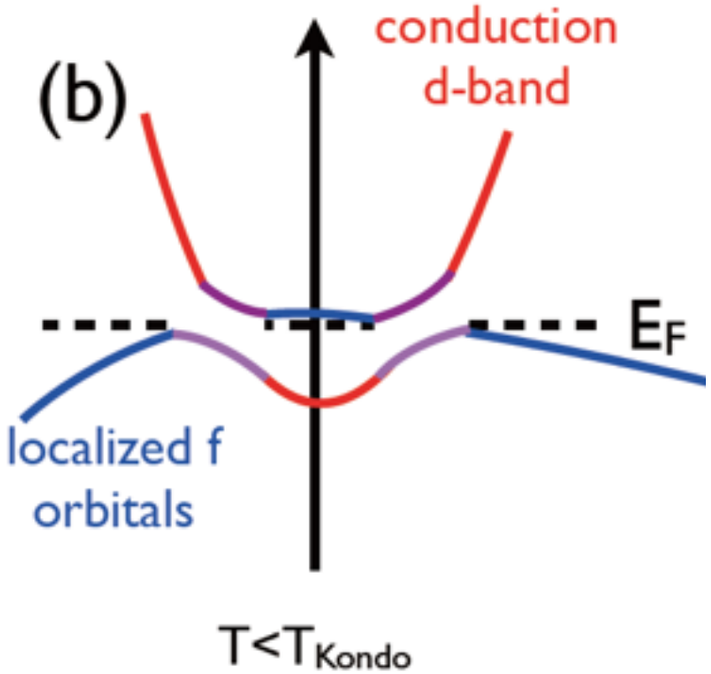
Previous ARPES result on SmB_6

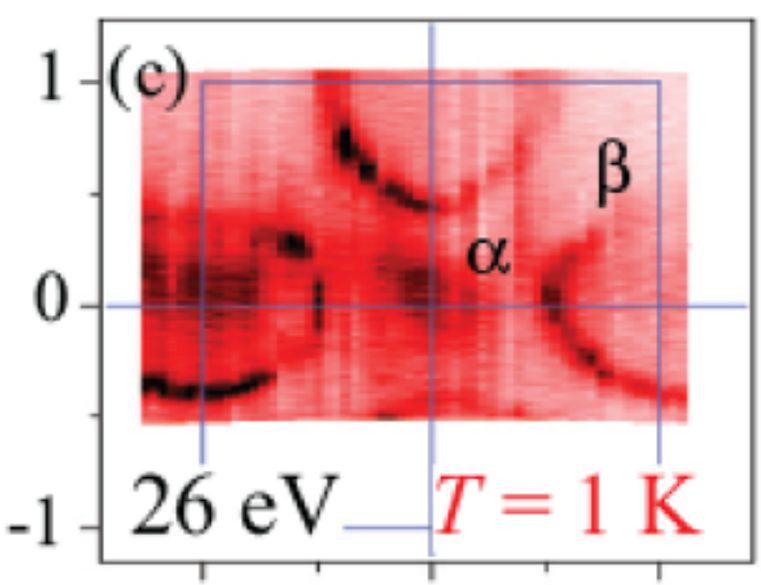
Previous ARPES result on SmB_6

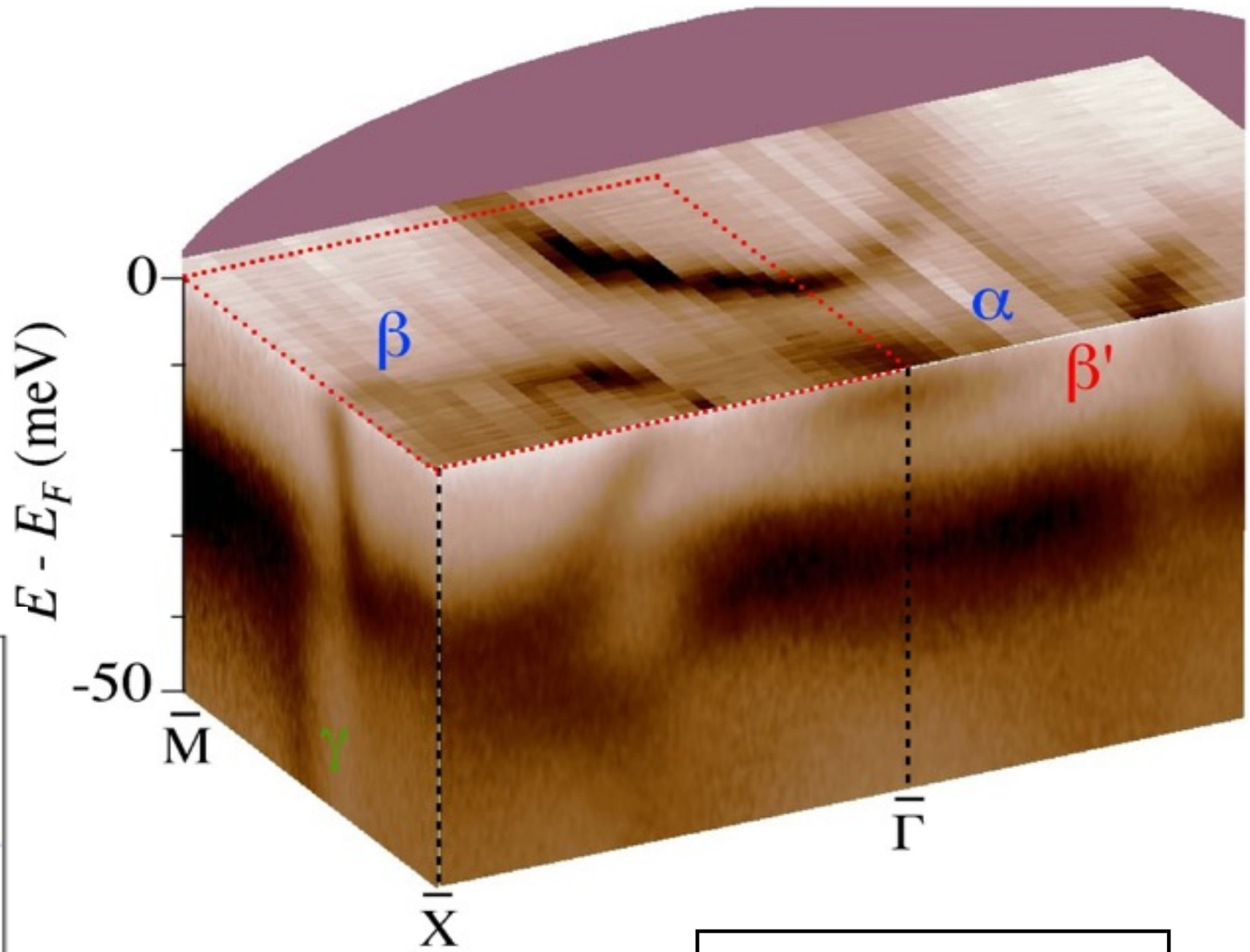


H. Miyazaki *et al.,* Phys. Rev. B 86, 075105 (2012).
J. D. Denlinger *et al.*, Physica B 281-282, 716 (2000).

In gap states



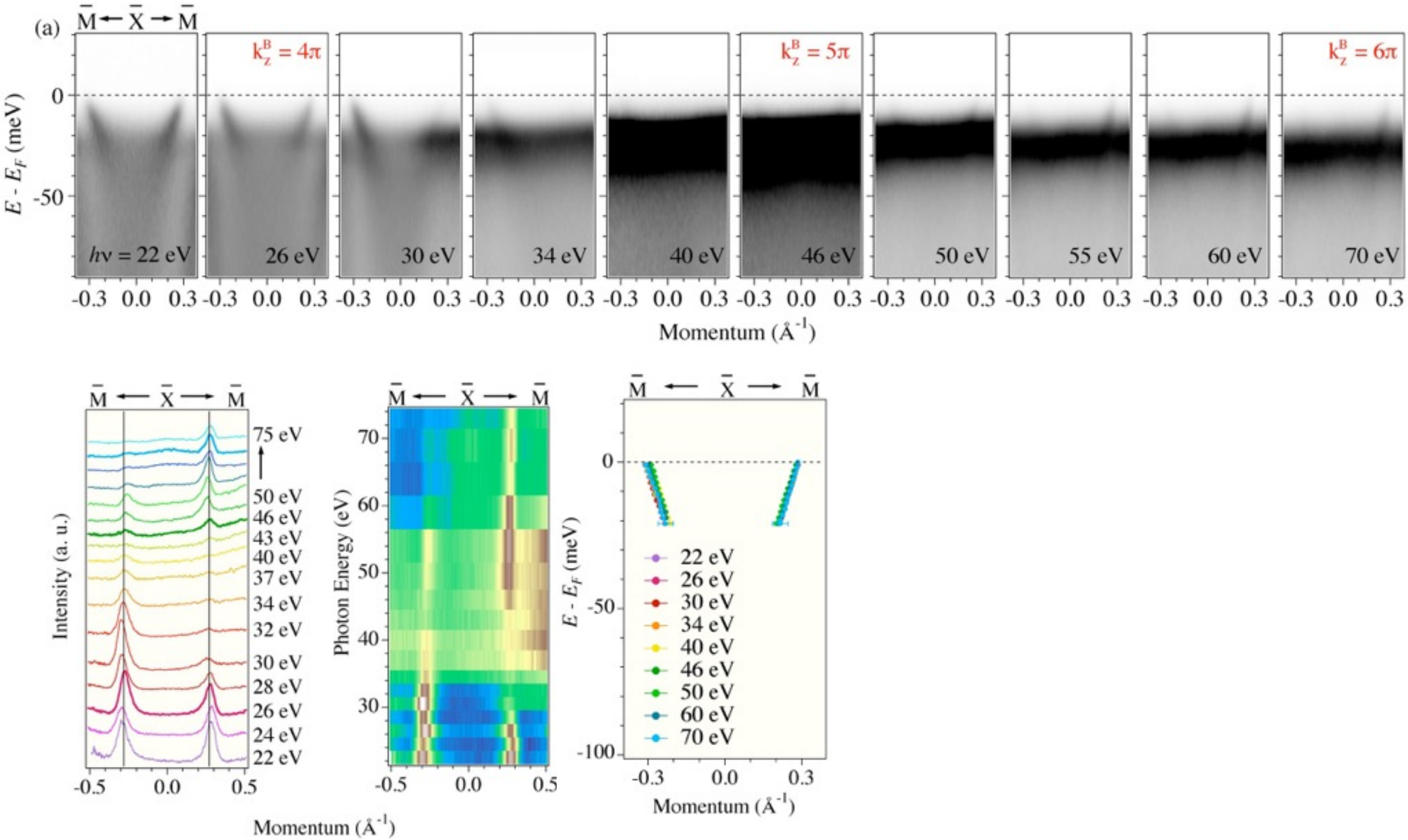




T = 1K, 26 eV ($k_z = 0$)

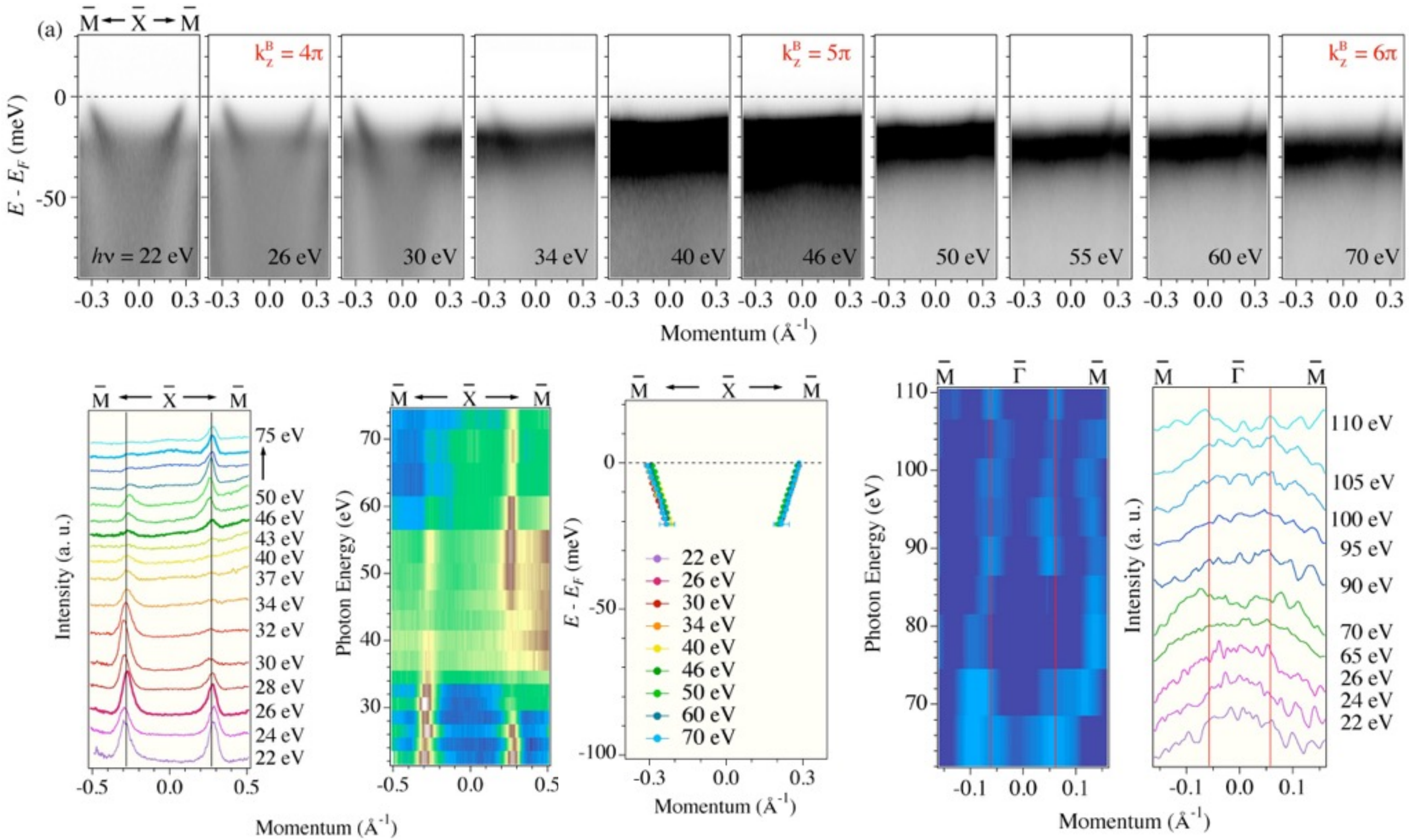
N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013), **Editors' Suggestion**.

Photon Energy dependence



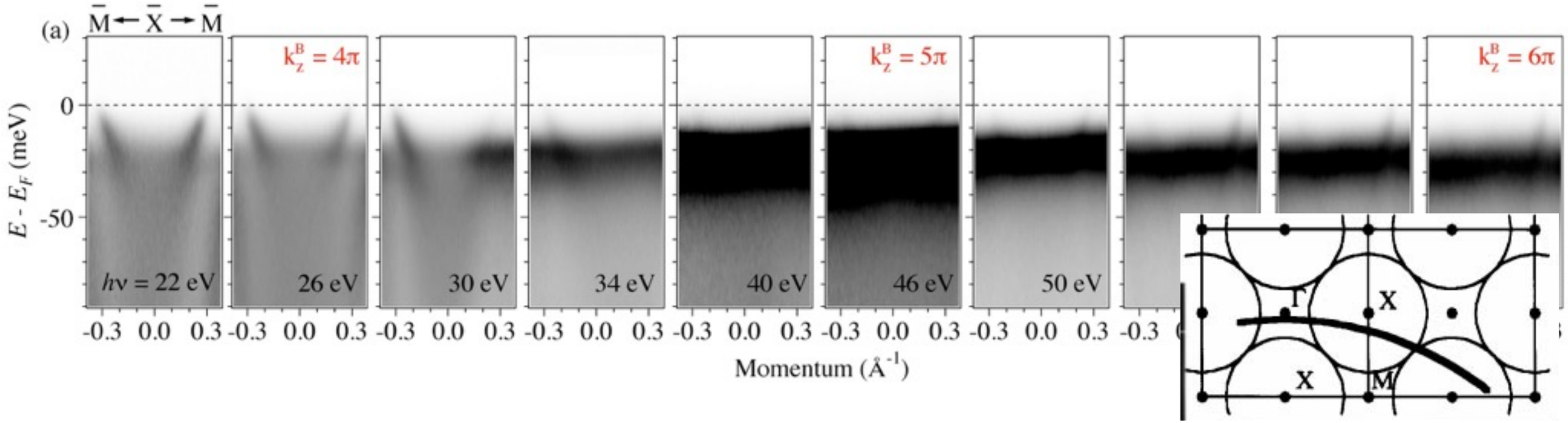
N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

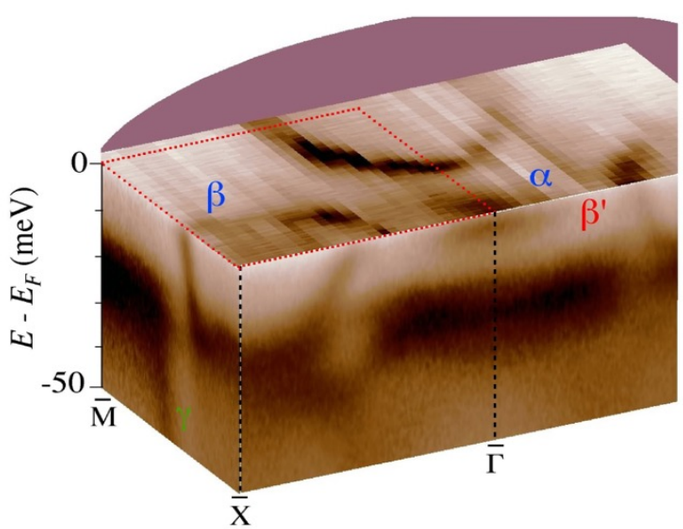
Photon Energy dependence



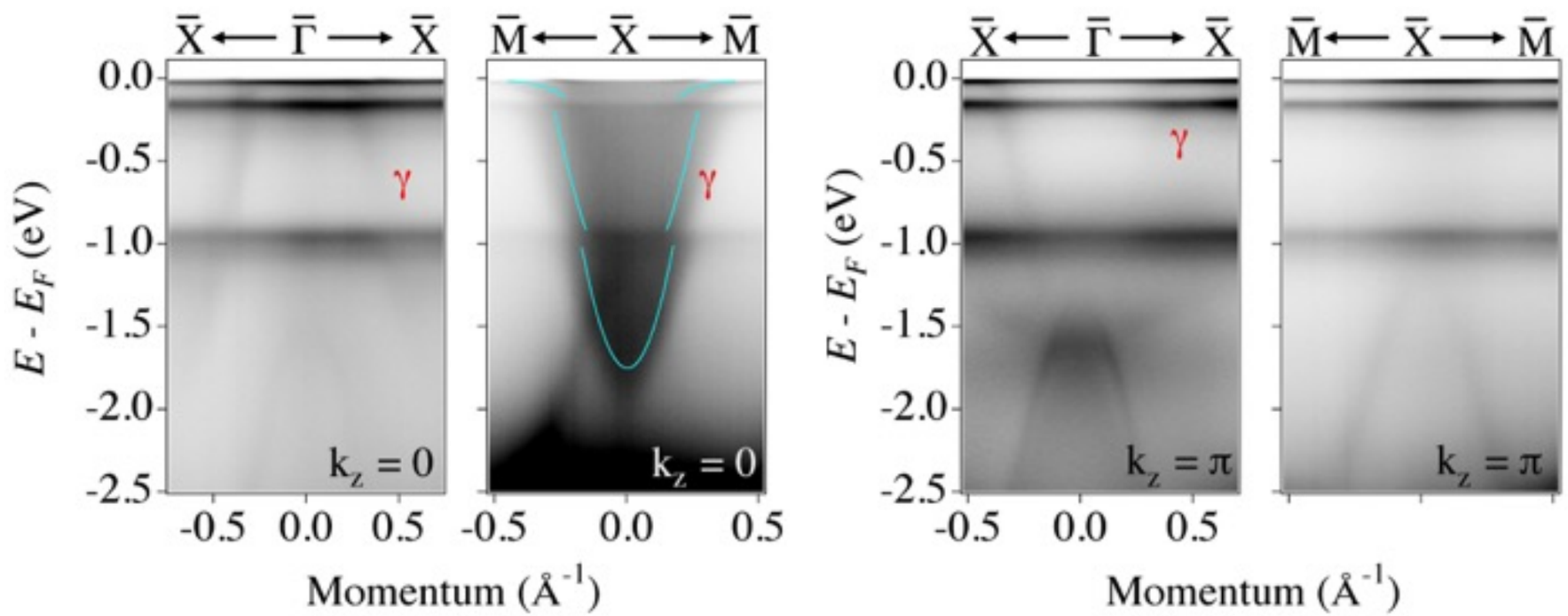
N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

Photon Energy dependence





T = 1K, 26 eV



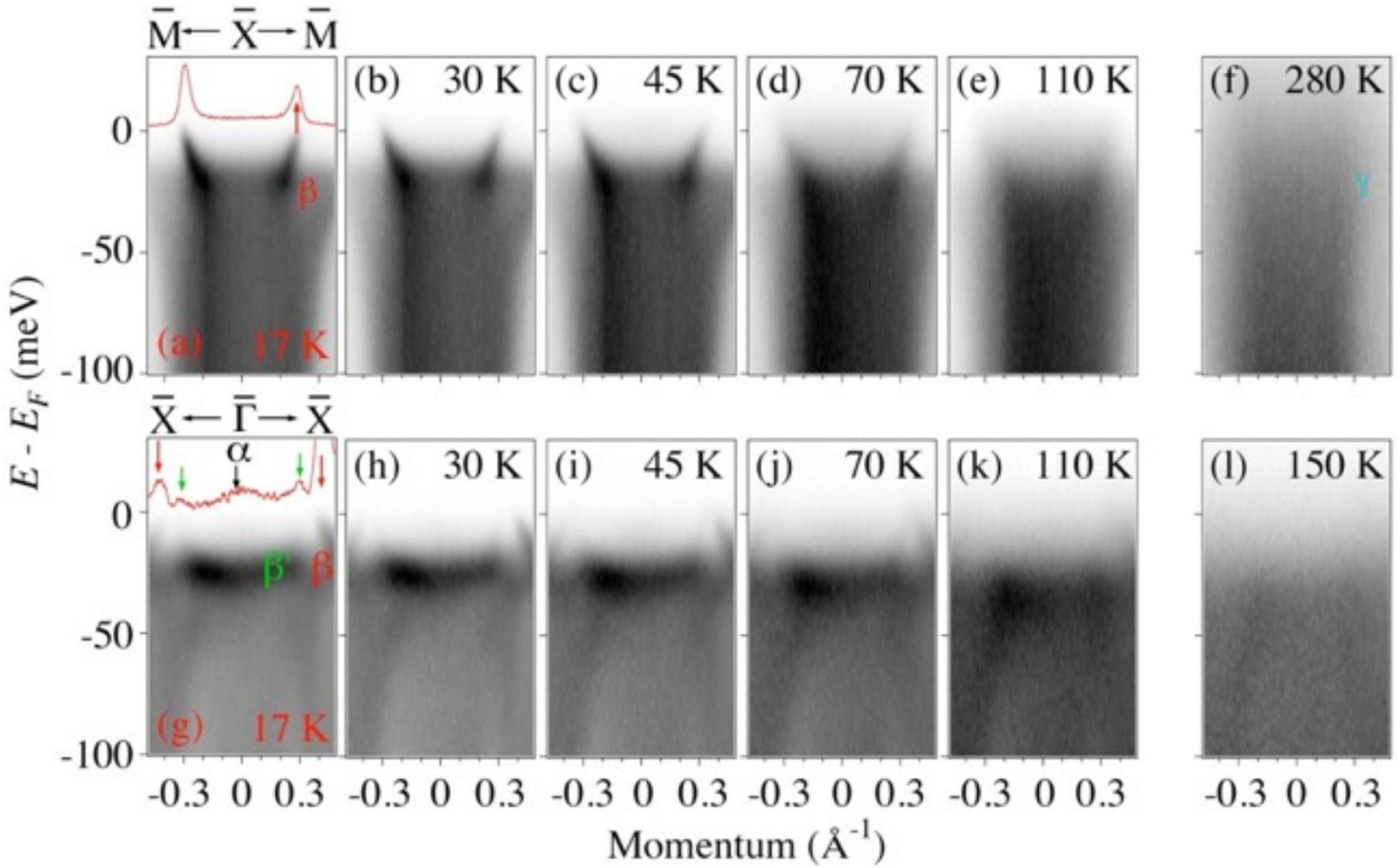
N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

Temperature Dependence

N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

J. D. Denlinger, J. W. Allen et al., arXiv. 1312.6637 (2013).

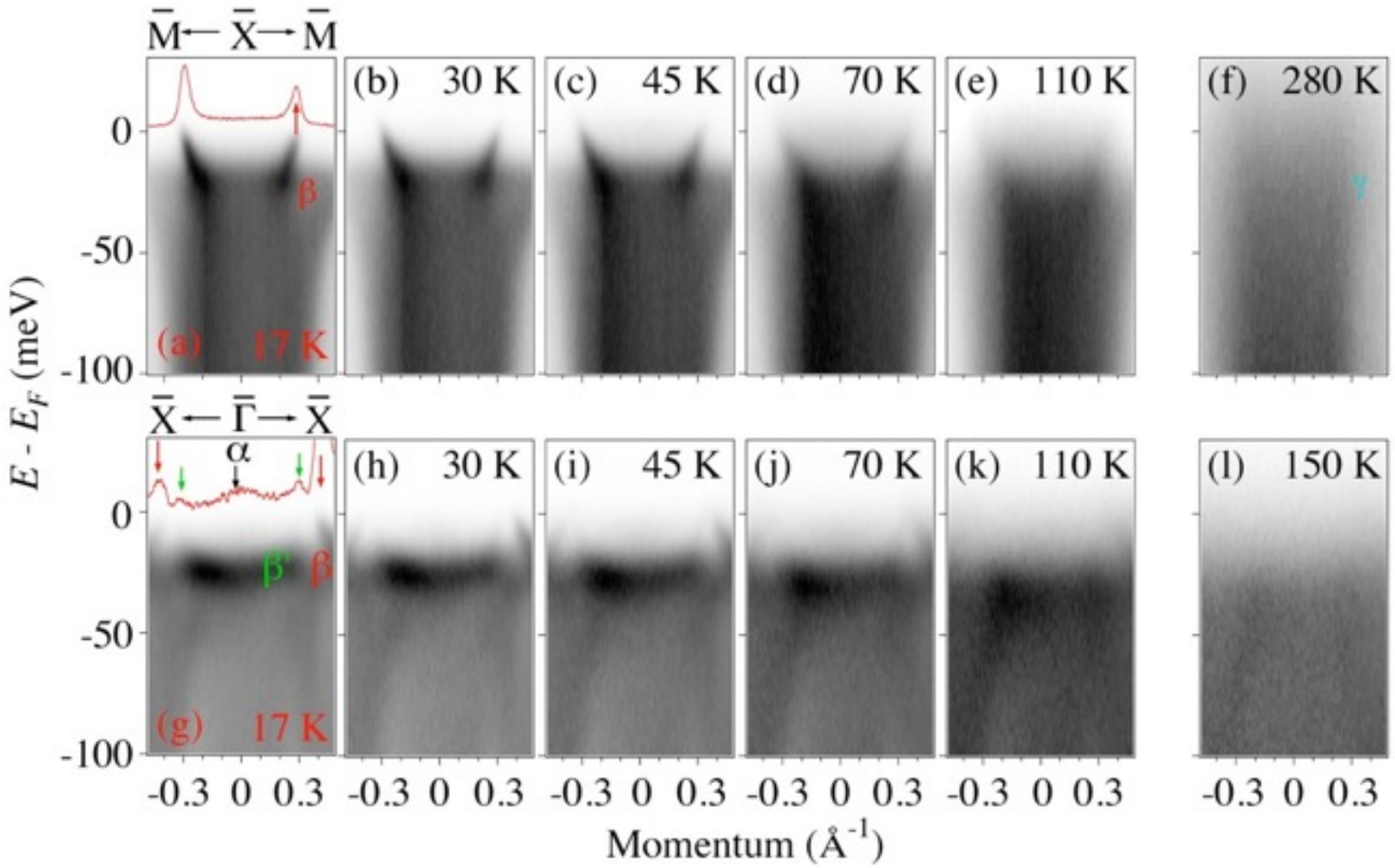
Temperature Dependence

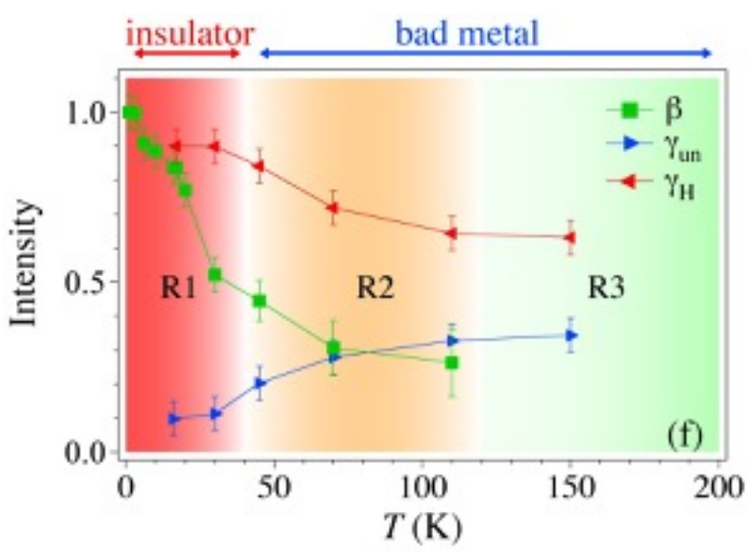


N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

J. D. Denlinger, J. W. Allen et al., arXiv. 1312.6637 (2013).

Temperature Dependence



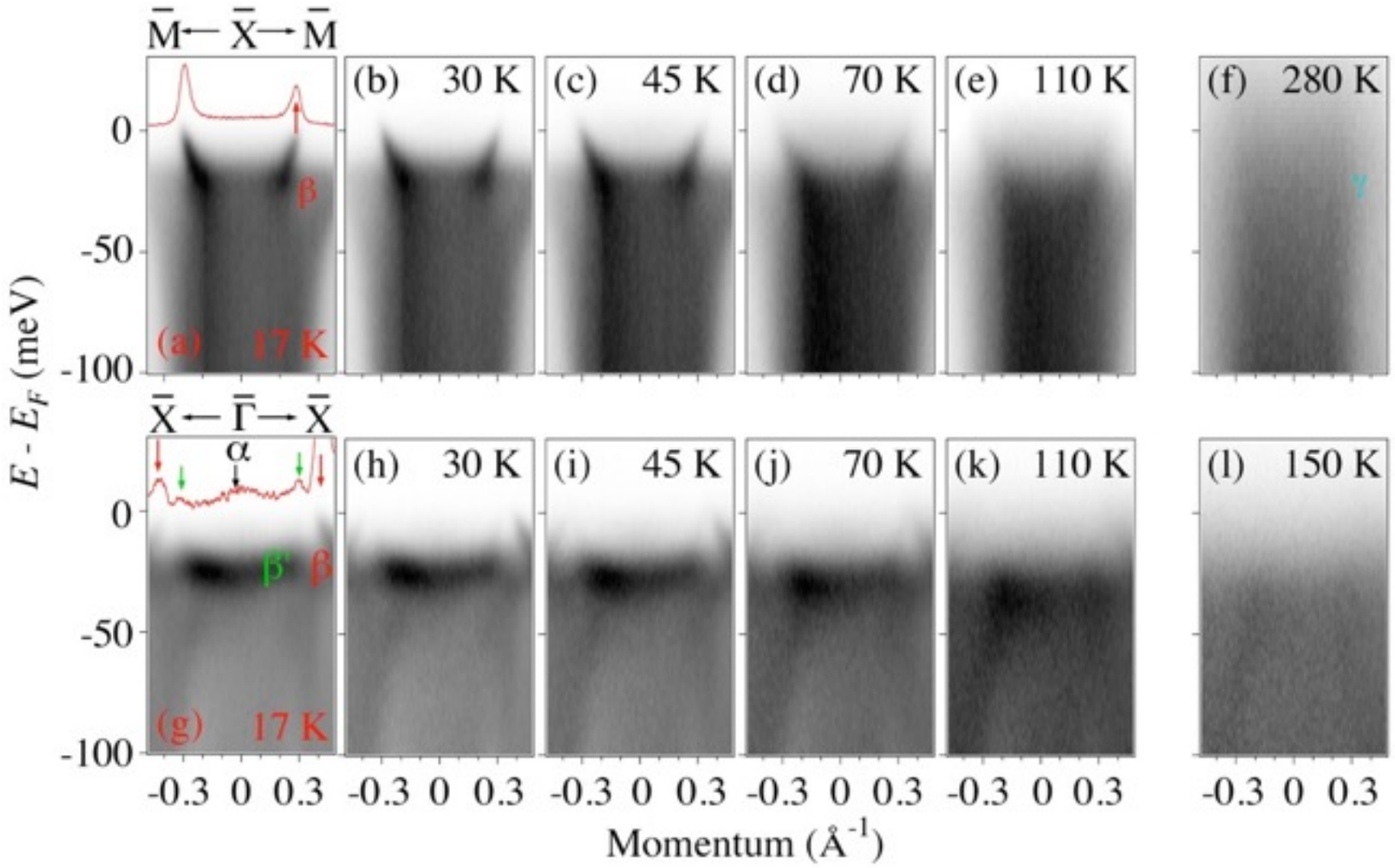


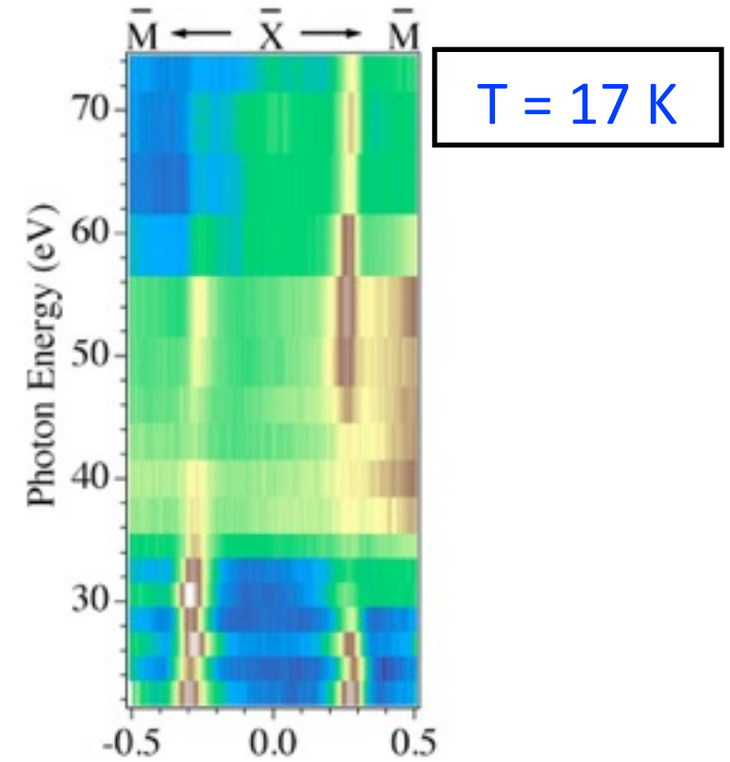
N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

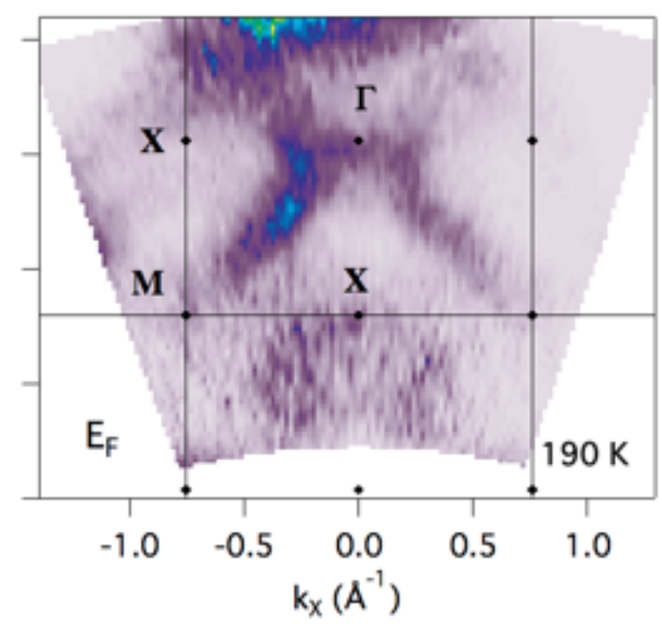
N. Xu *et al.*, Phy. Rev. B **90**, 085148 (2014).

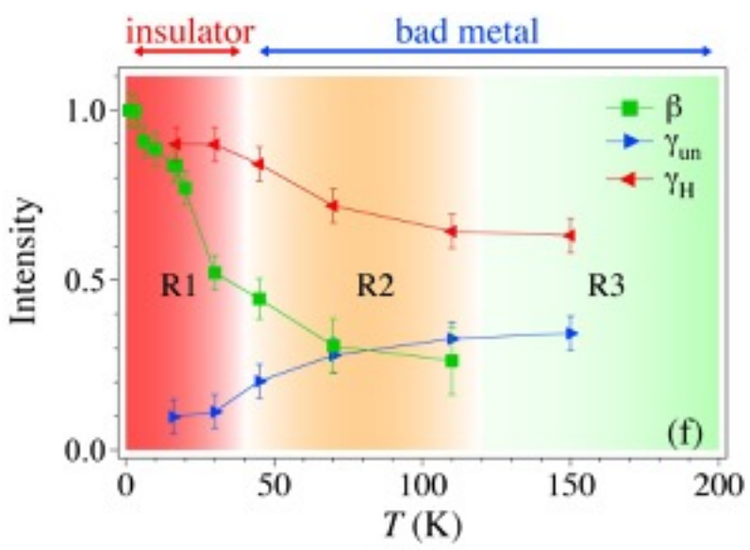
J. D. Denlinger, J. W. Allen et al., arXiv. 1312.6637 (2013).

Temperature Dependence









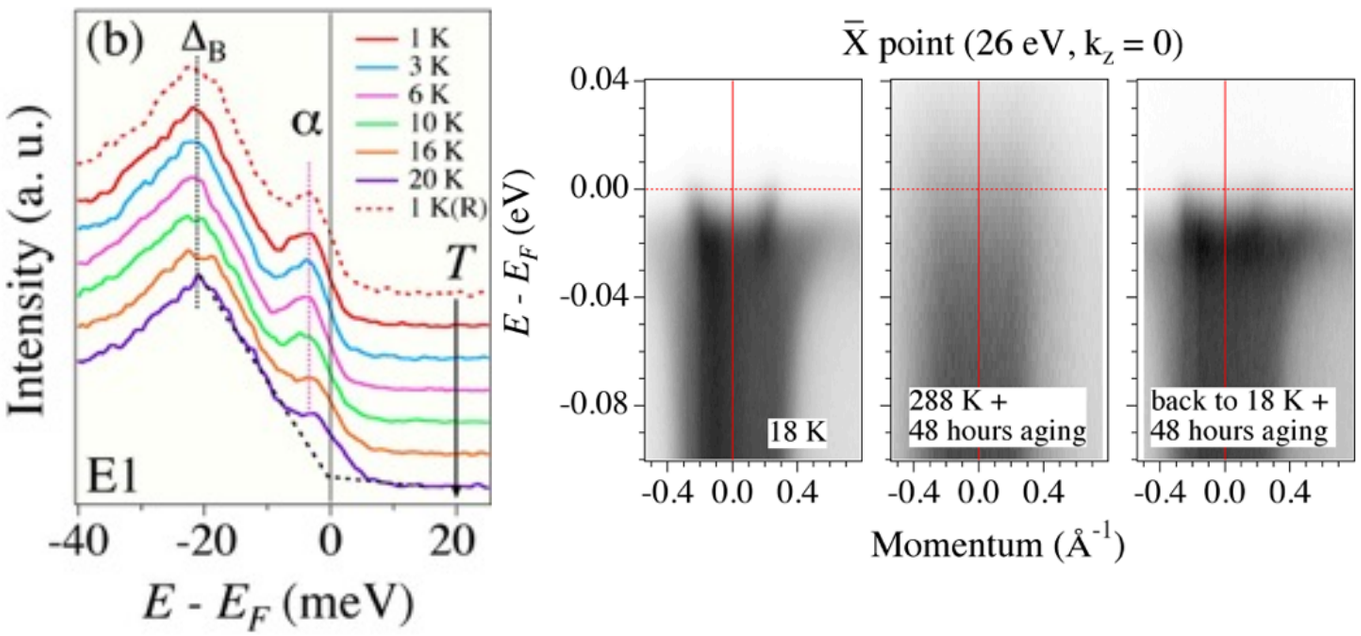
N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

N. Xu *et al.*, Phy. Rev. B **90**, 085148 (2014).

J. D. Denlinger, J. W. Allen et al., arXiv. 1312.6637 (2013).

Protected SS

Robust from thermo-cycle

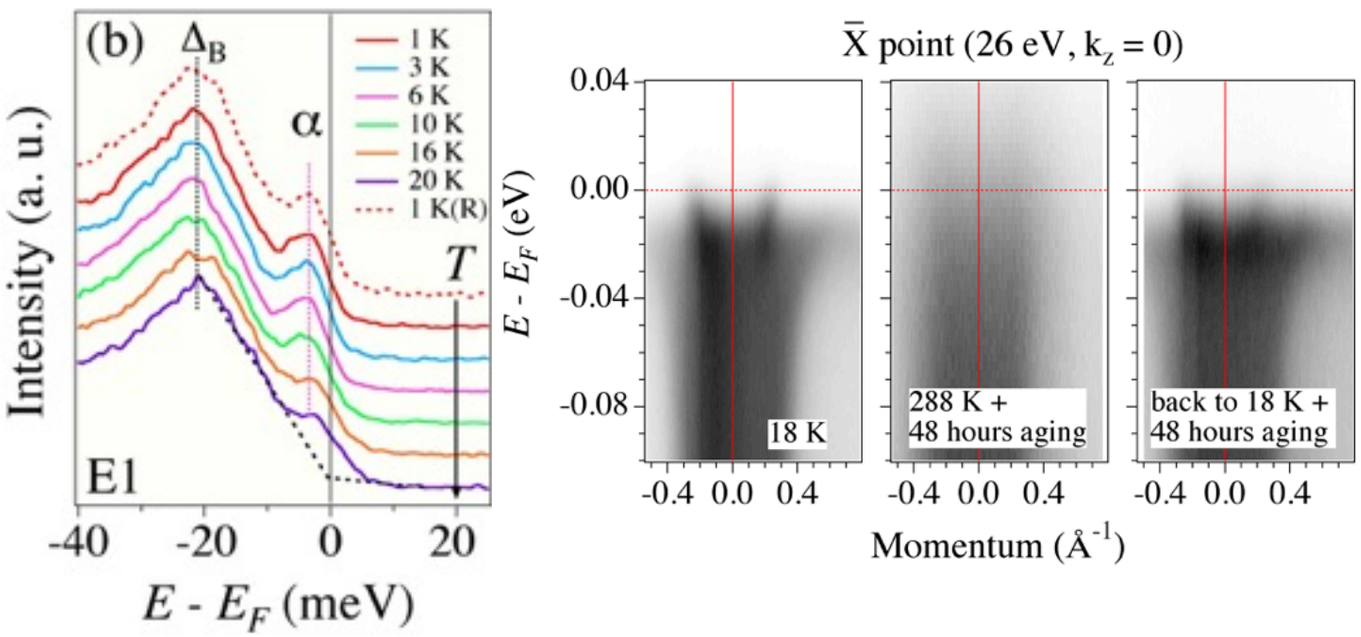


N. Xu *et al.*, Phy. Rev. B **88**, 121102(R) (2013).

Robust from surface conditions

Protected SS

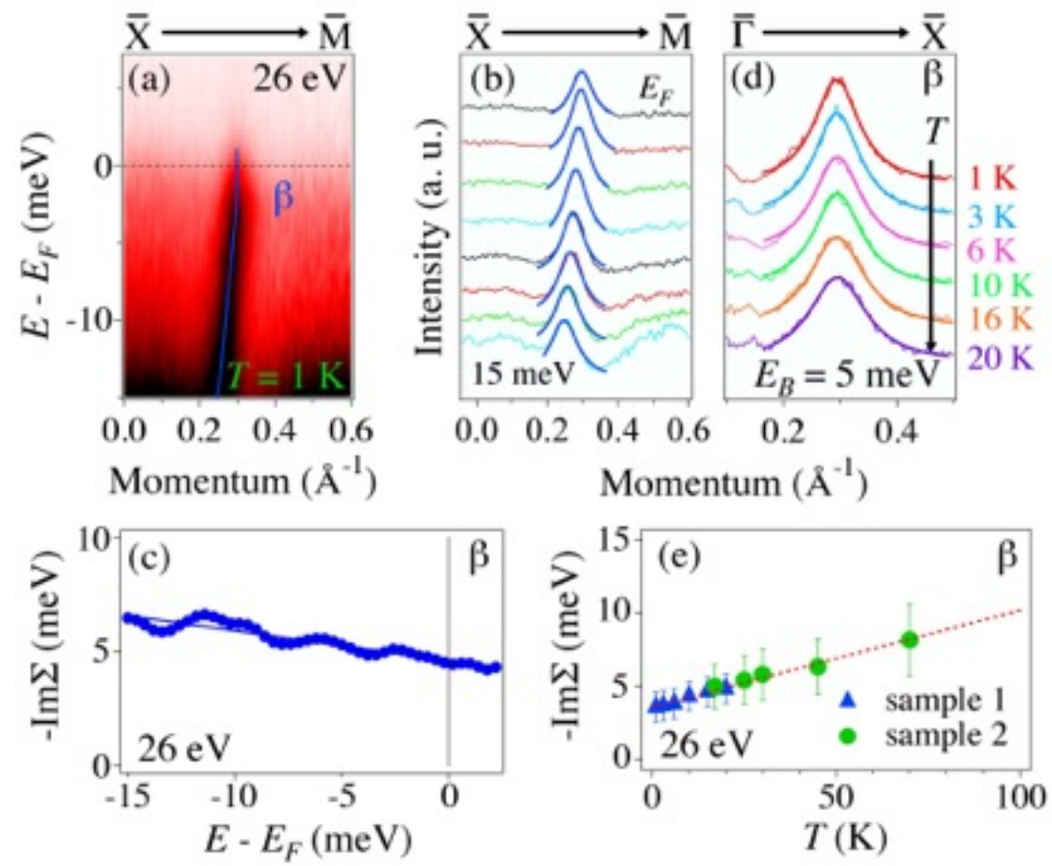
Robust from thermo-cycle



N. Xu *et al.*, Phy. Rev. B **88**, 121102(R) (2013).

Robust from surface conditions

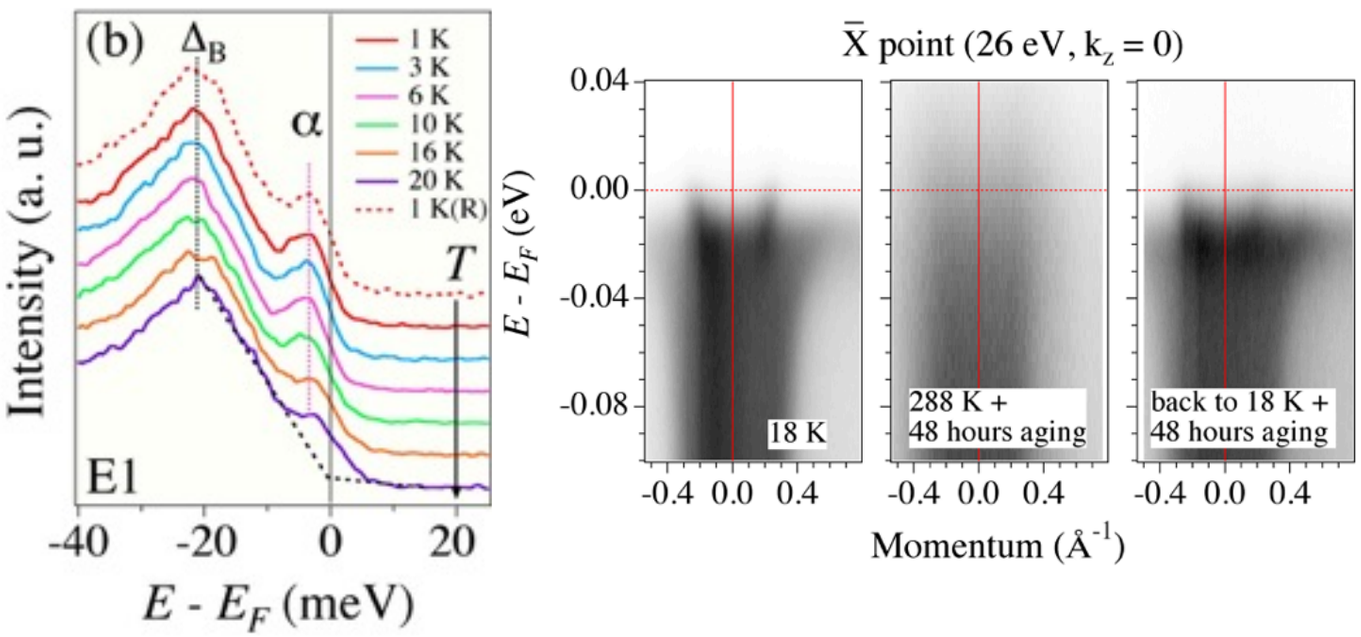
Suppressed scattering rate



N. Xu *et al.*, Phy. Rev. B **90**, 085148 (2014).

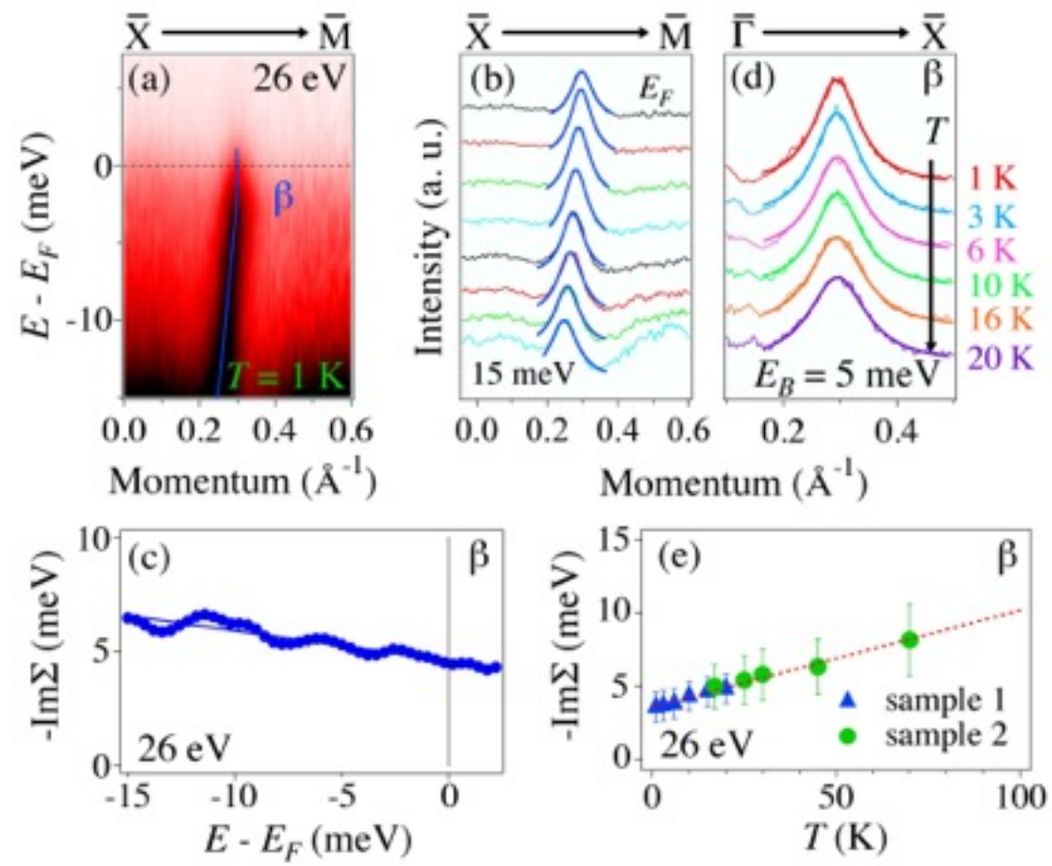
Protected SS

Robust from thermo-cycle



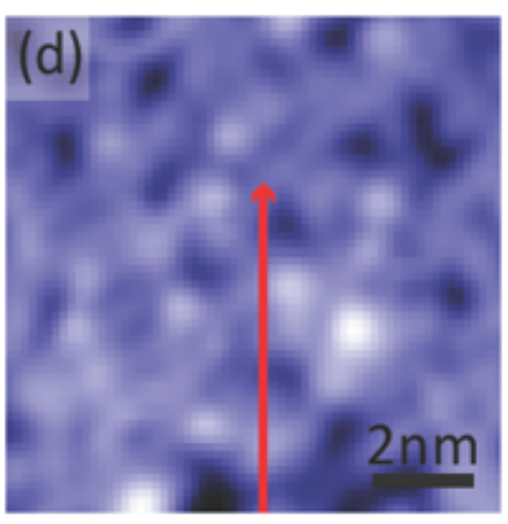
N. Xu *et al.*, Phy. Rev. B **88**, 121102(R) (2013).

Suppressed scattering rate



N. Xu *et al.*, Phy. Rev. B **90**, 085148 (2014).

Robust from surface conditions



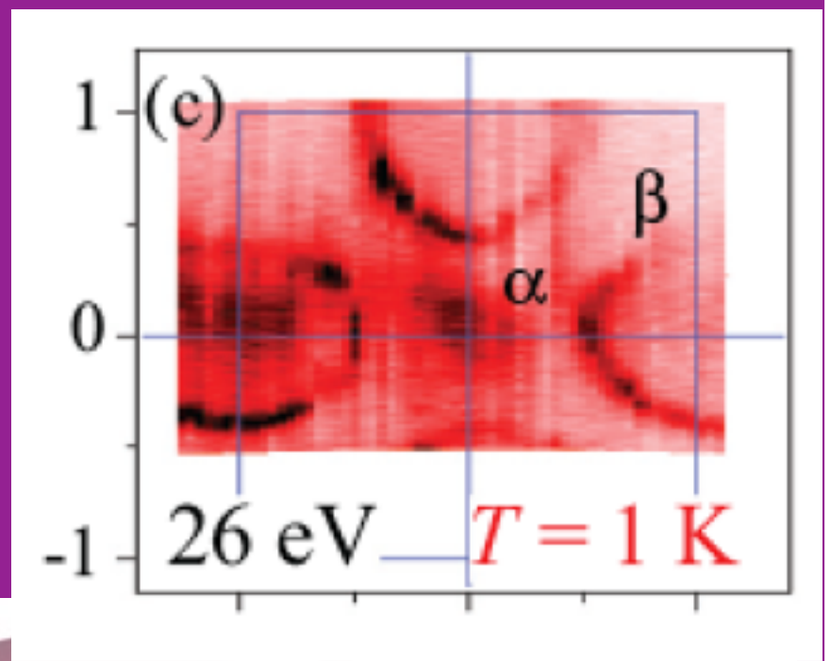
Sahana Rößler *et al.*, PNAS 111, 4798 (2014)

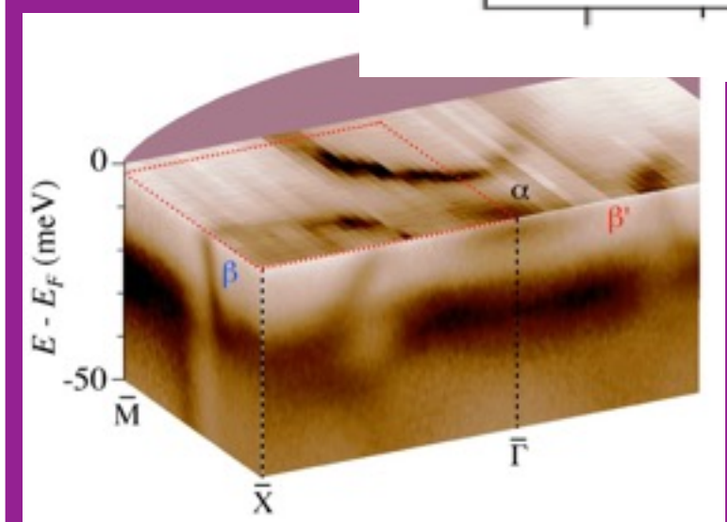
Wei Ruan *et al.*, PRL 112, 136401 (2014)

Michael M. Yee *et al.*, arXiv: 1308.1085 (2013)

Comparison of electronic structure with theory

SmB_6

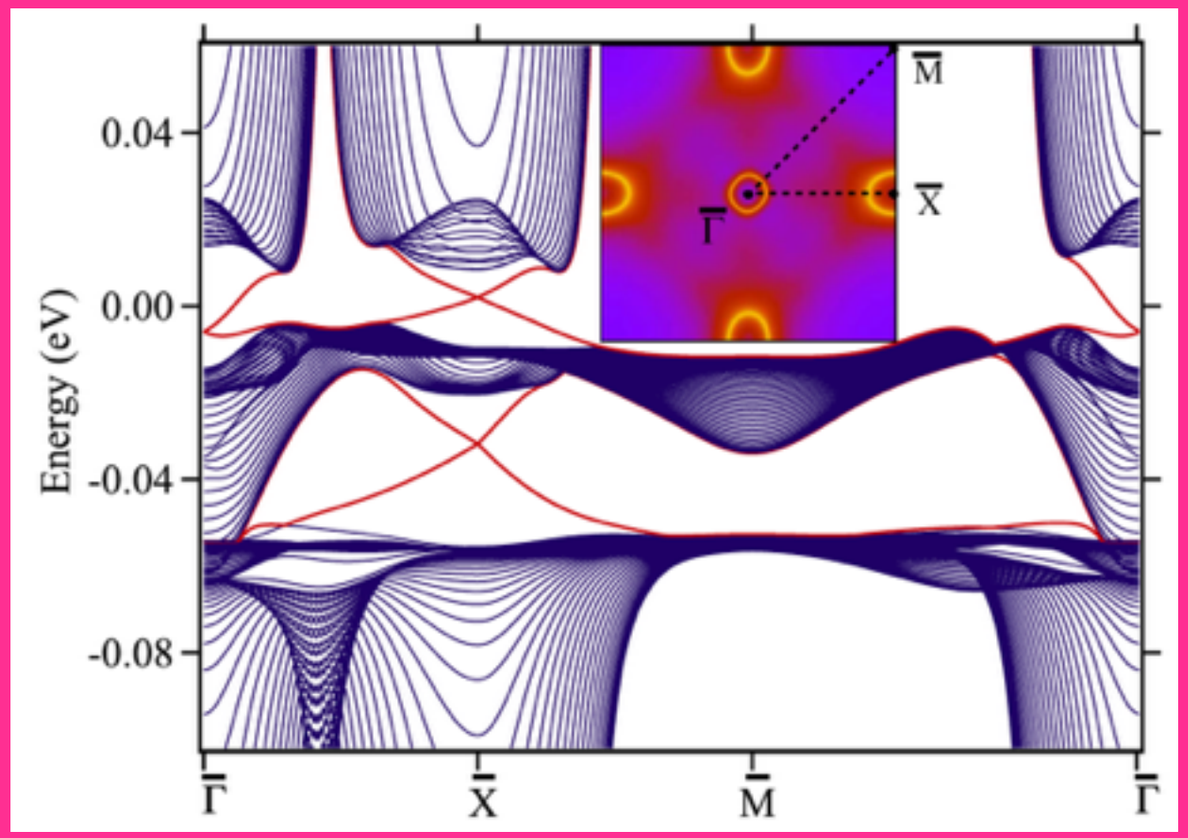




Three SS pockets centered at $\bar{\Gamma}$/ $\bar{X}$ point

N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

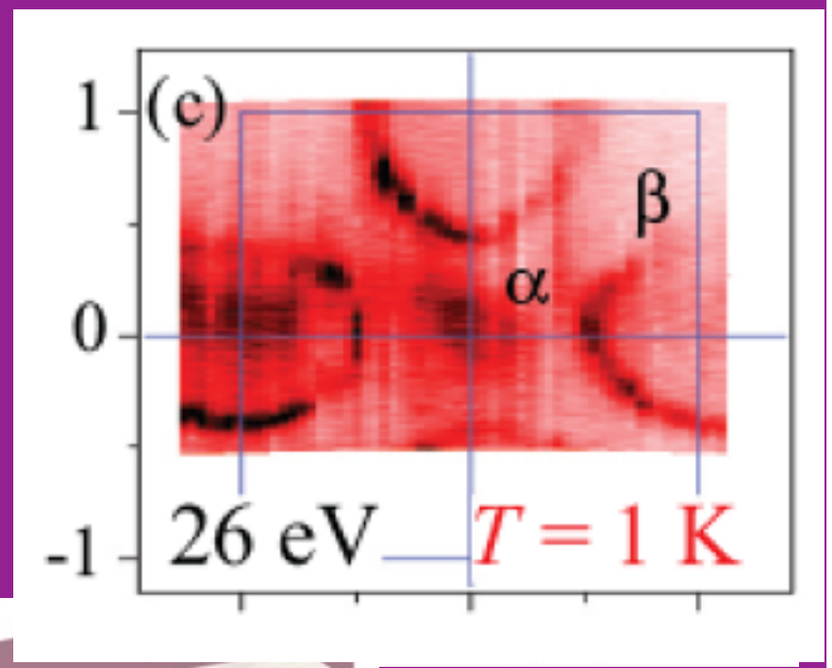
Theoretical prediction of TKI

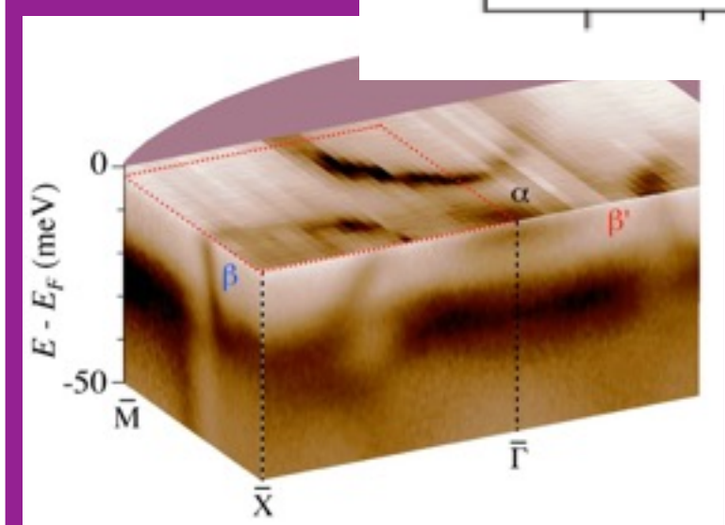


F. Lu, J. Zhao, H. Weng, X. Dai and Z. Fang, Phys. Rev. Lett. **110**, 096401 (2013).

Comparison of electronic structure with theory

SmB_6

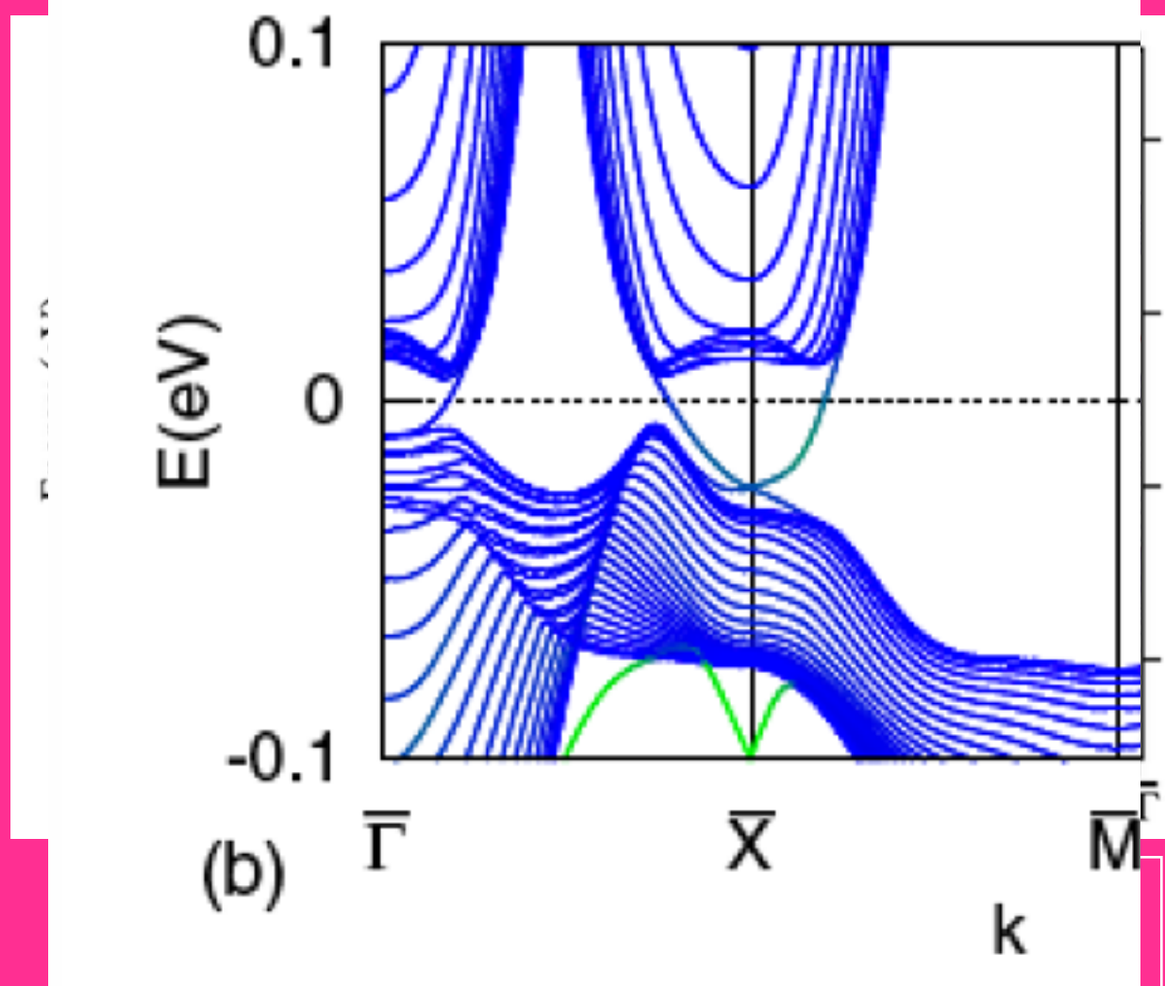




Three SS pockets centered at $\bar{\Gamma}$/ $\bar{X}$ point

N. Xu *et al.*, Phy. Rev. B 88, 121102(R) (2013)

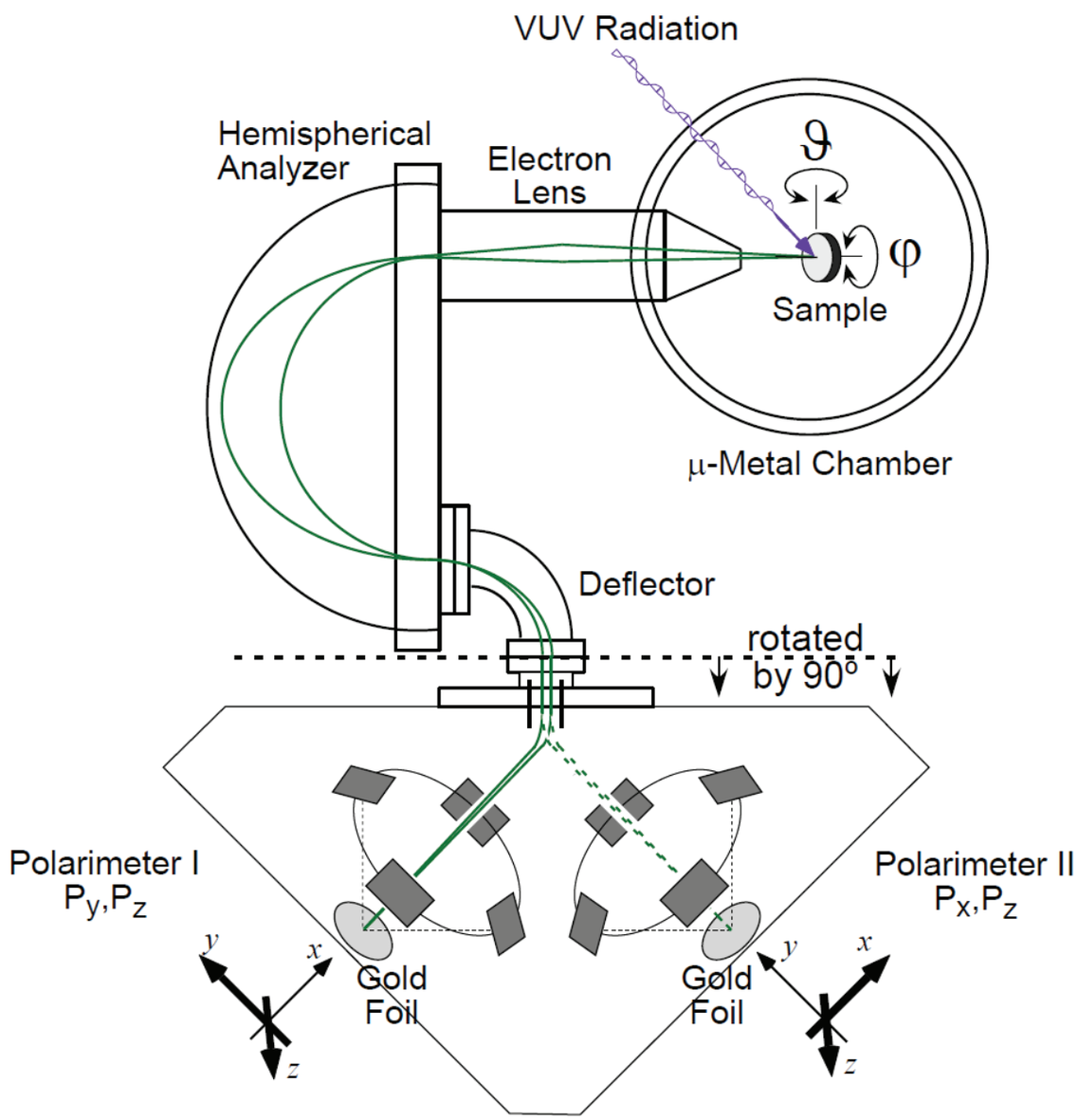
Theoretical prediction of TKI



Pier Paolo Baruselli and Matthias Vojta, PRB 90, 201106(R) (2014)

SARPES

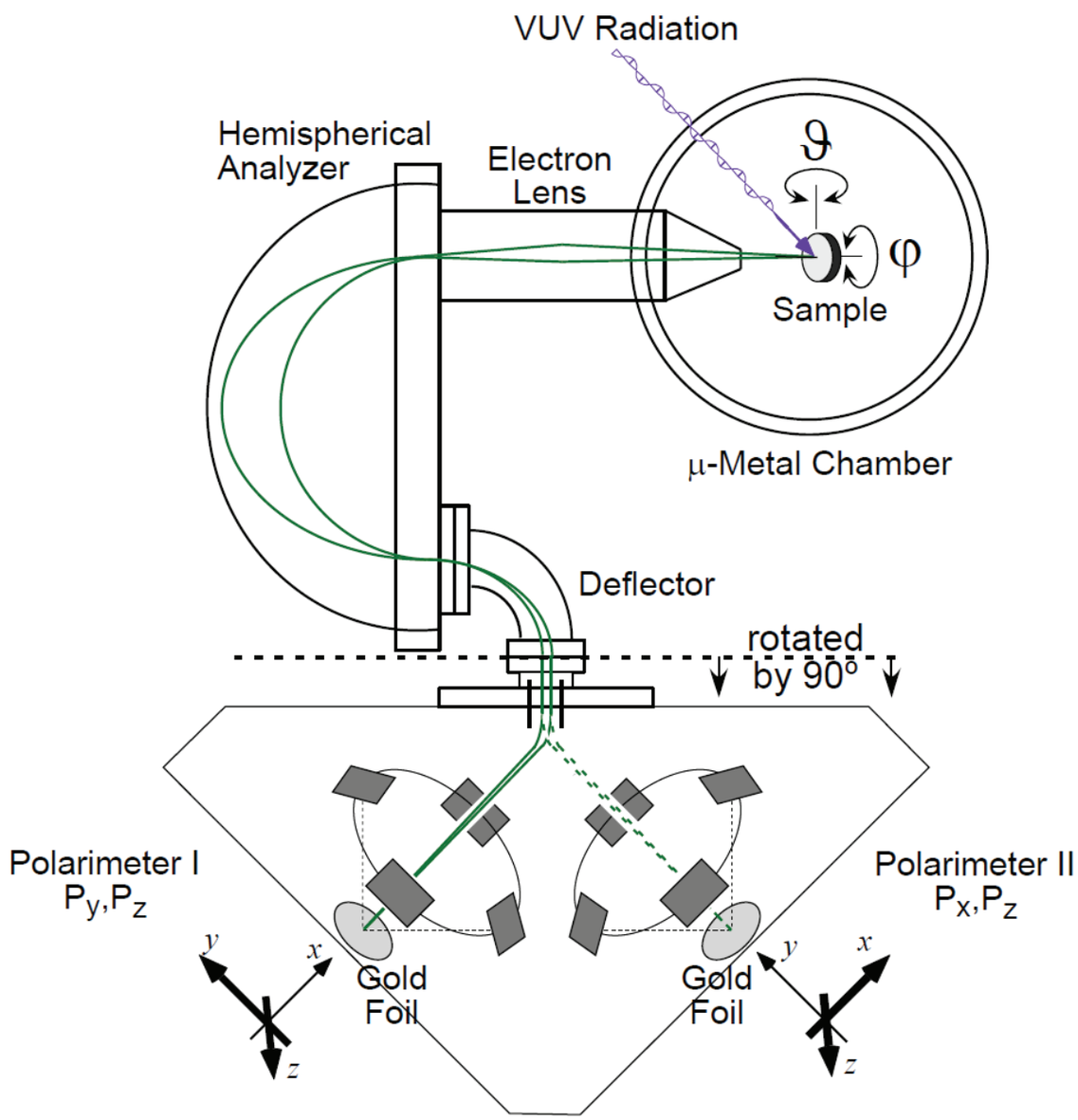
COPHEE = The **CO**mplete **PH**oto**E**mission **E**xperiment

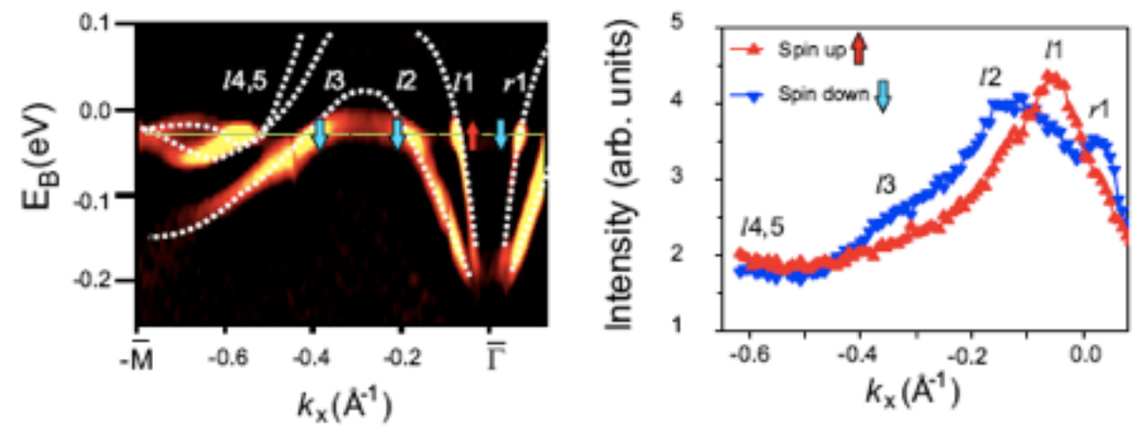


Access to "all" quantum numbers of the electron: energy, momentum (3D) and spin (3D)

SARPES

COPHEE = The **CO**mplete **PH**oto**E**mission **E**xperiment



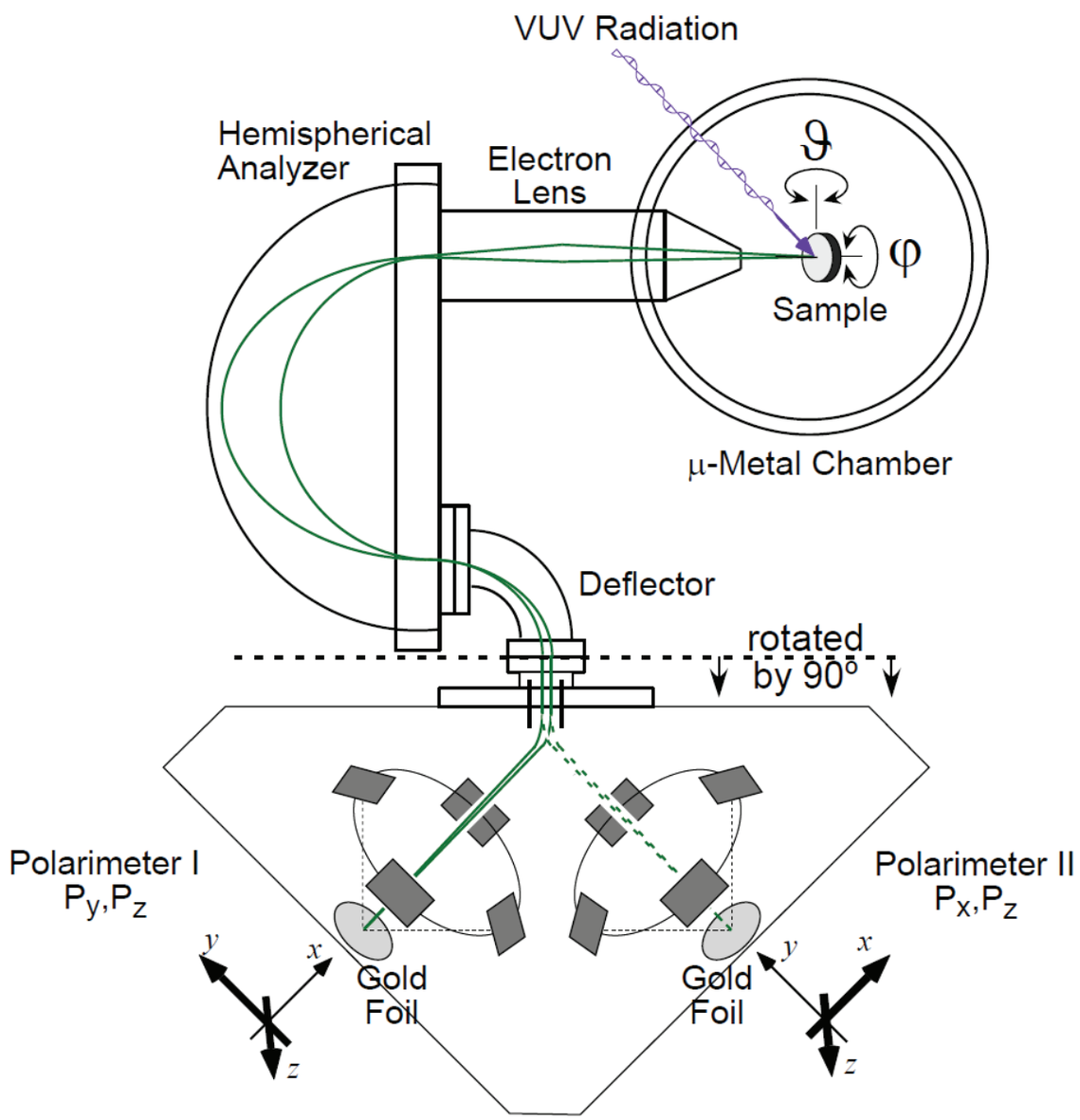


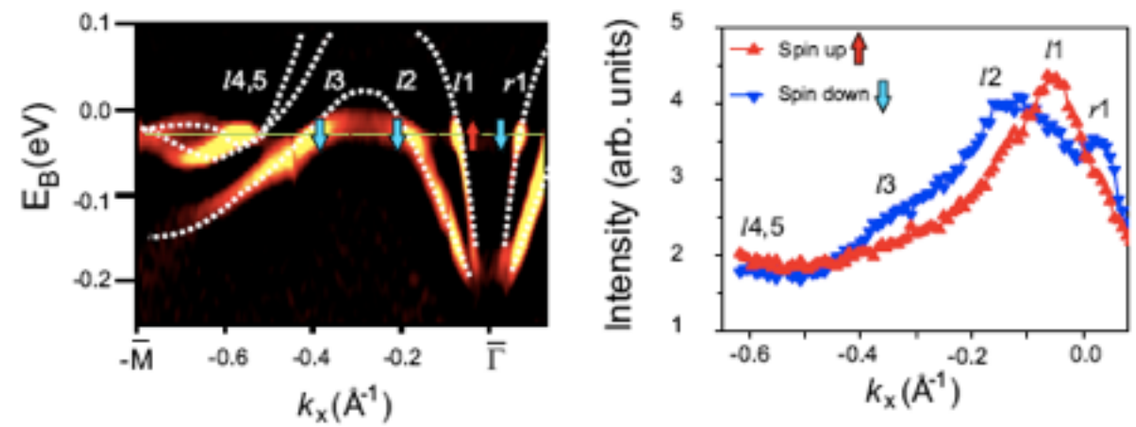
D. Hsieh et al., Science 323, 919 (2009)

Access to "all" quantum numbers of the electron: energy, momentum (3D) and spin (3D)

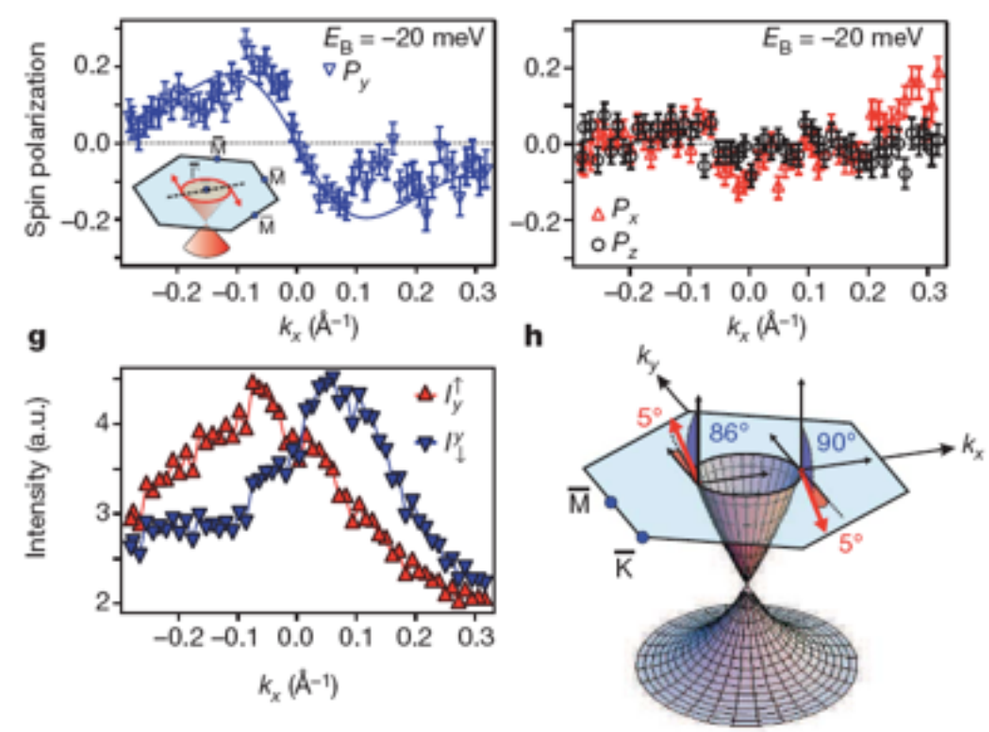
SARPES

COPHEE = The **CO**mplete **PH**oto**E**mission **E**xperiment





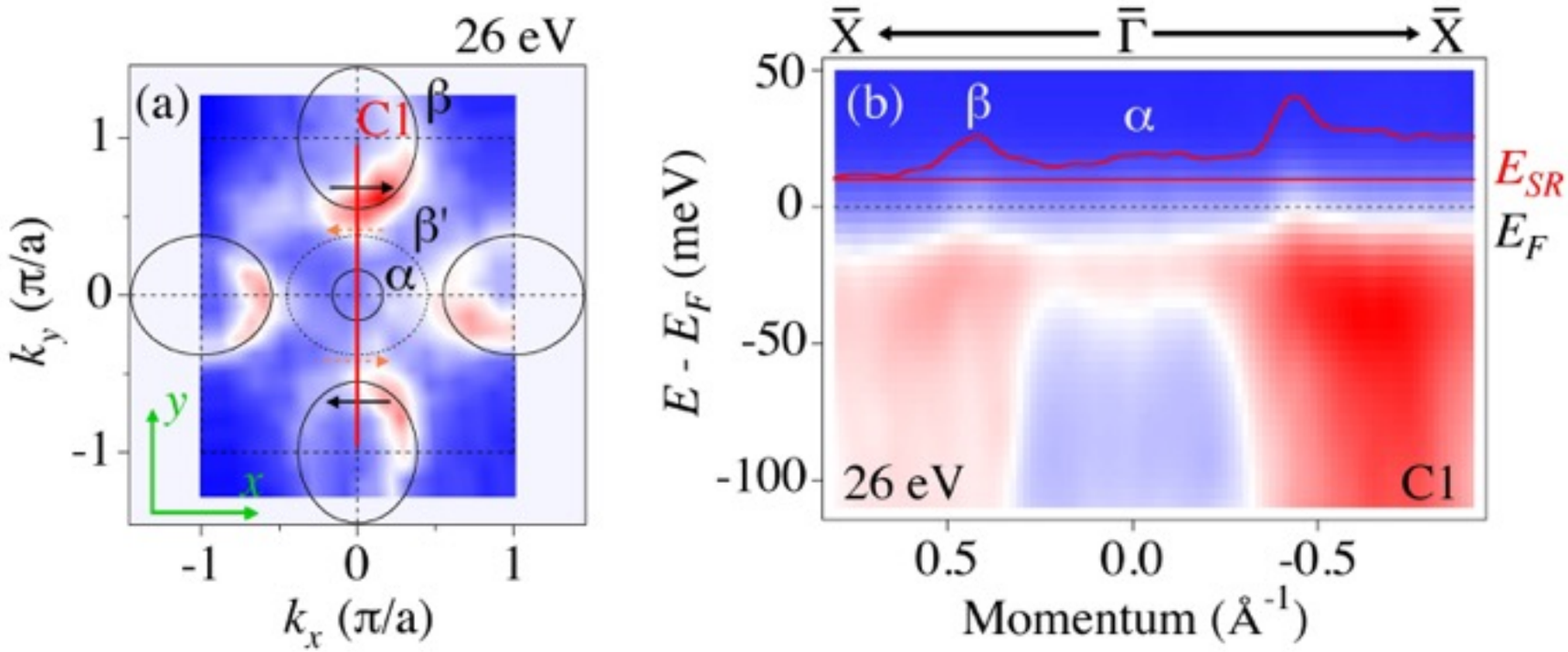
D. Hsieh et al., Science 323, 919 (2009)



D. Hsieh et al., Nature 460,1101 (2009)

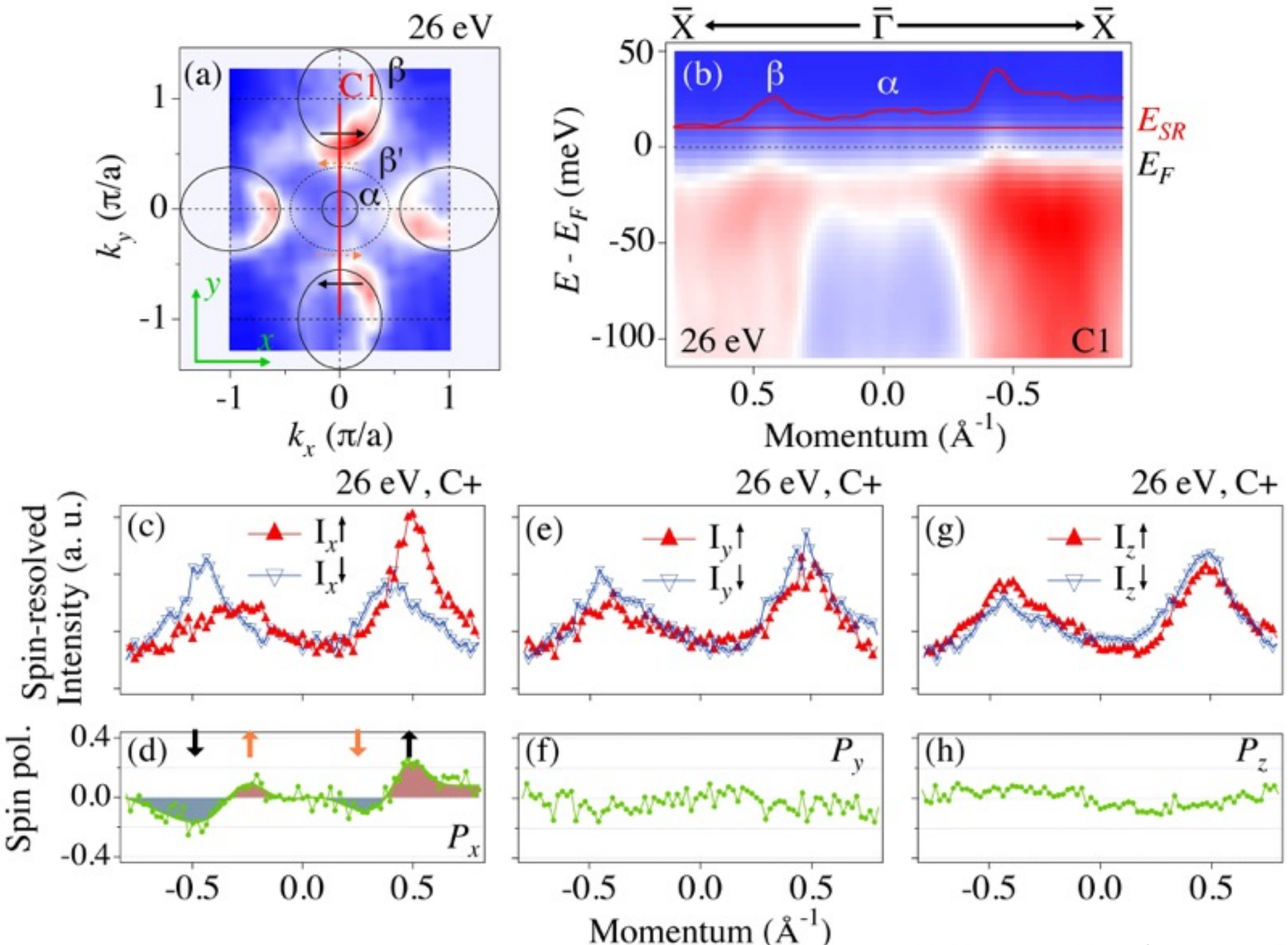
Access to "all" quantum numbers of the electron: energy, momentum (3D) and spin (3D)

Spin polarization



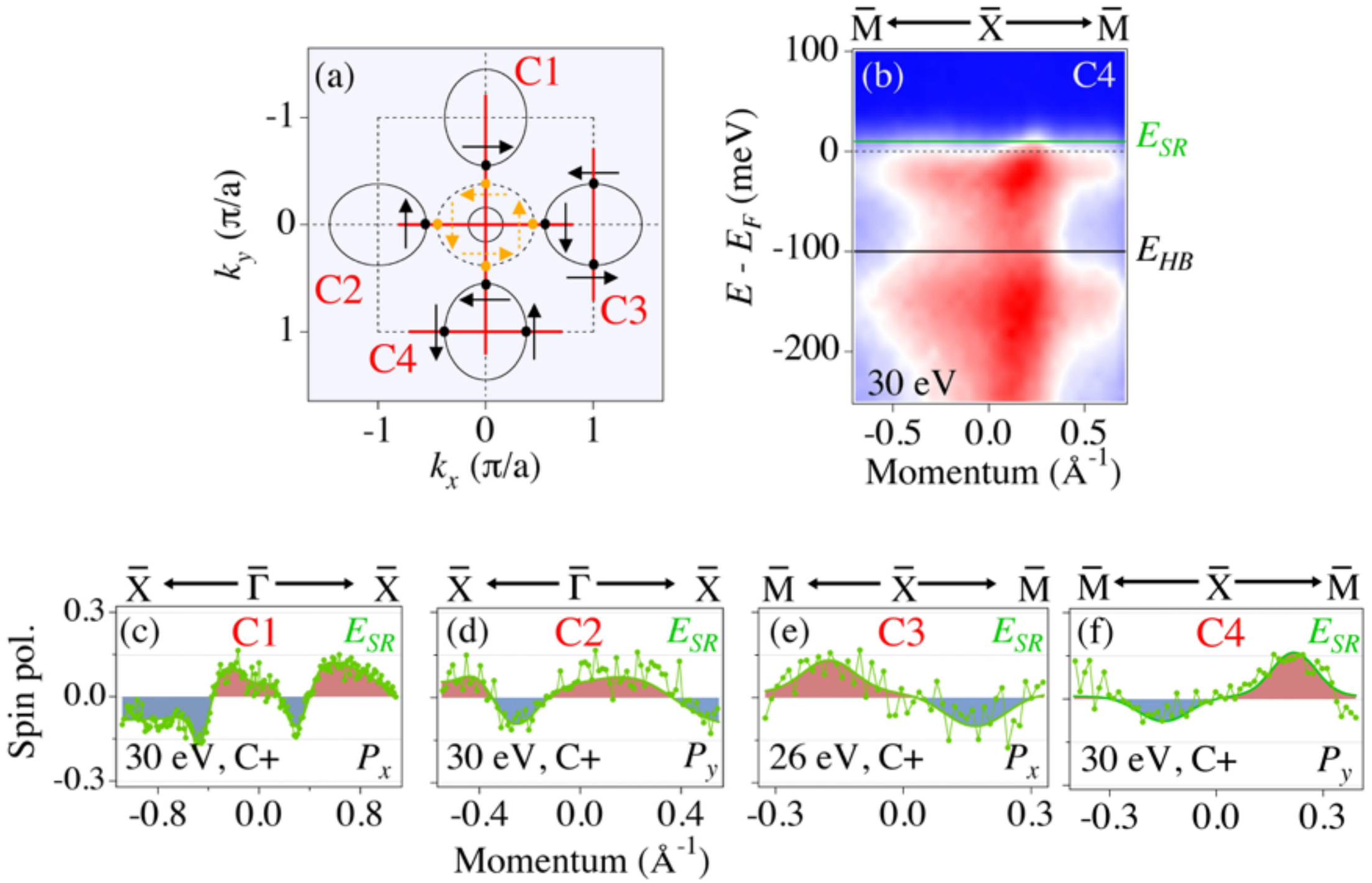
N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

Spin polarization



N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

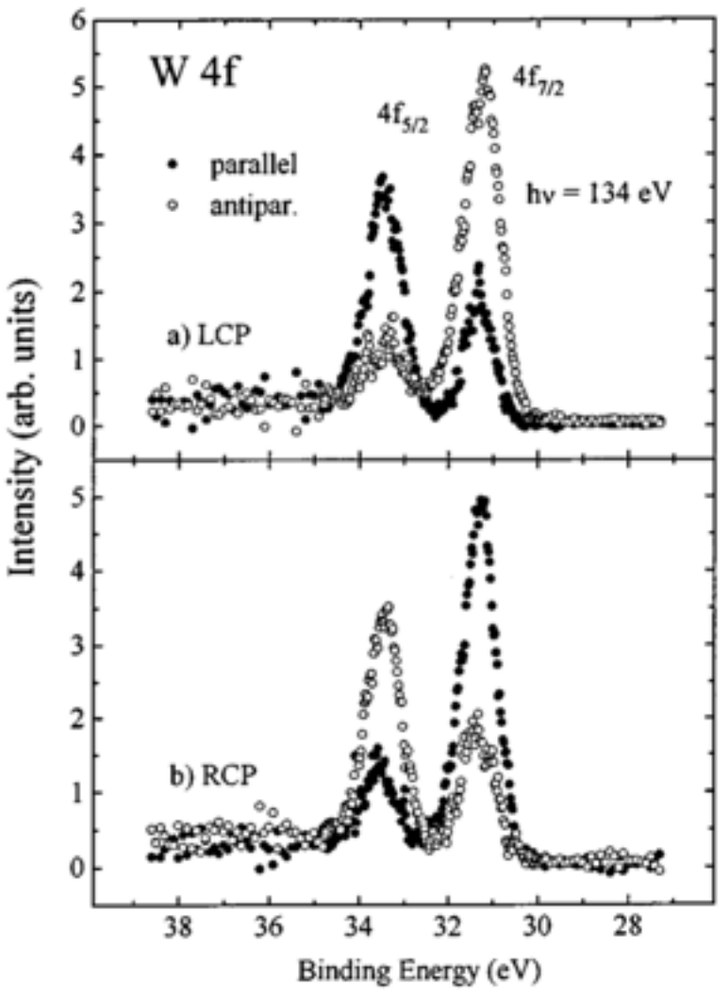
Spin texture



N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

Spin signal from Photoemission effect

core levels of non-magnetic materials

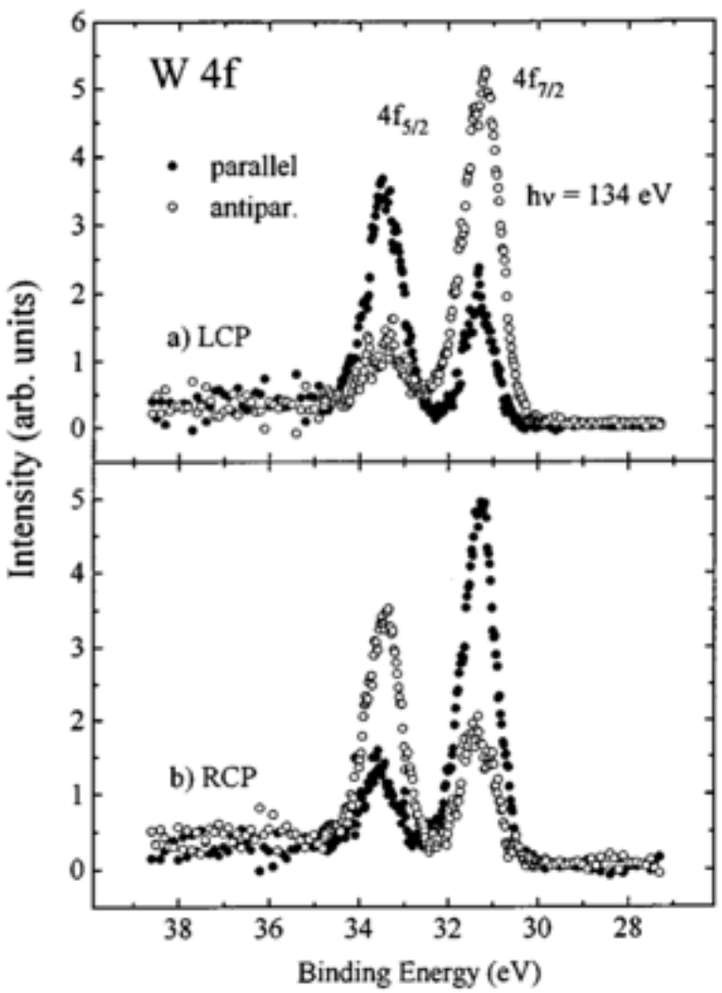


K. Starke *et al.,* Phys. Rev. B 53, 10544 (1996).

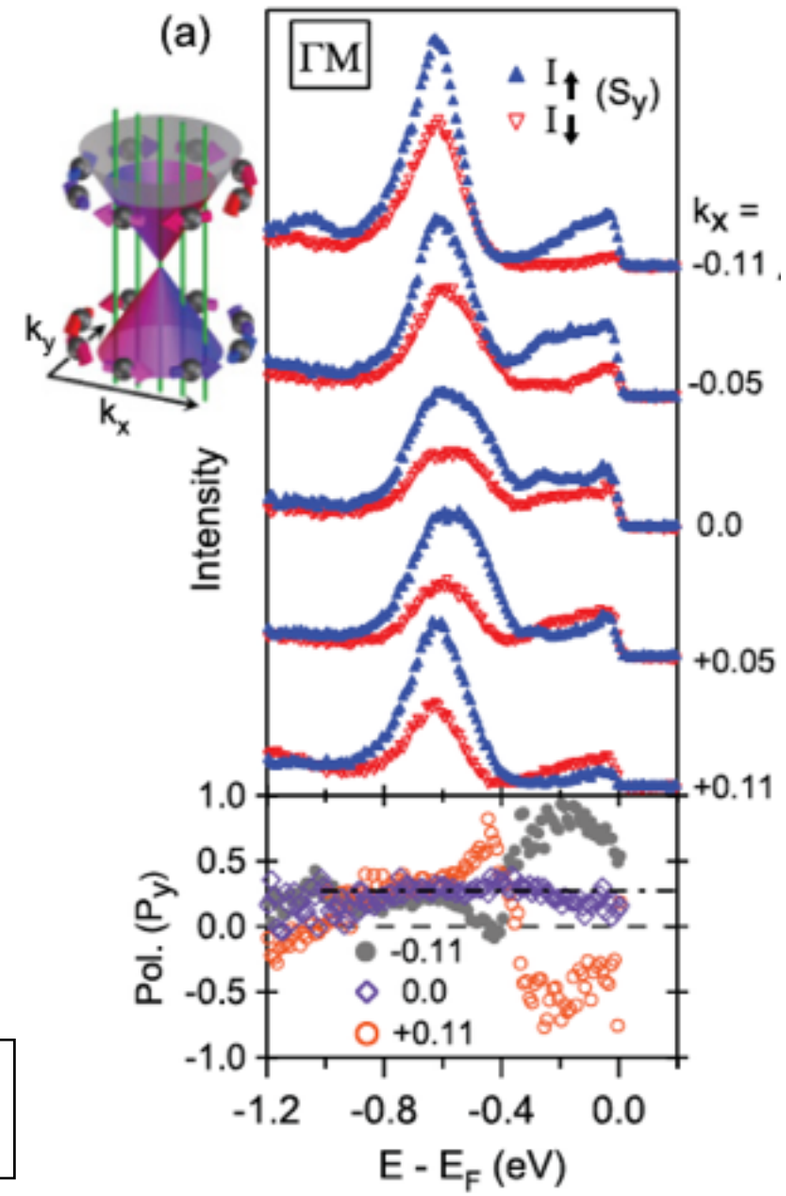
Spin signal from Photoemission effect

core levels of non-magnetic materials

bulk valence bands of topological insulators



K. Starke *et al.,* Phys. Rev. B 53, 10544 (1996).



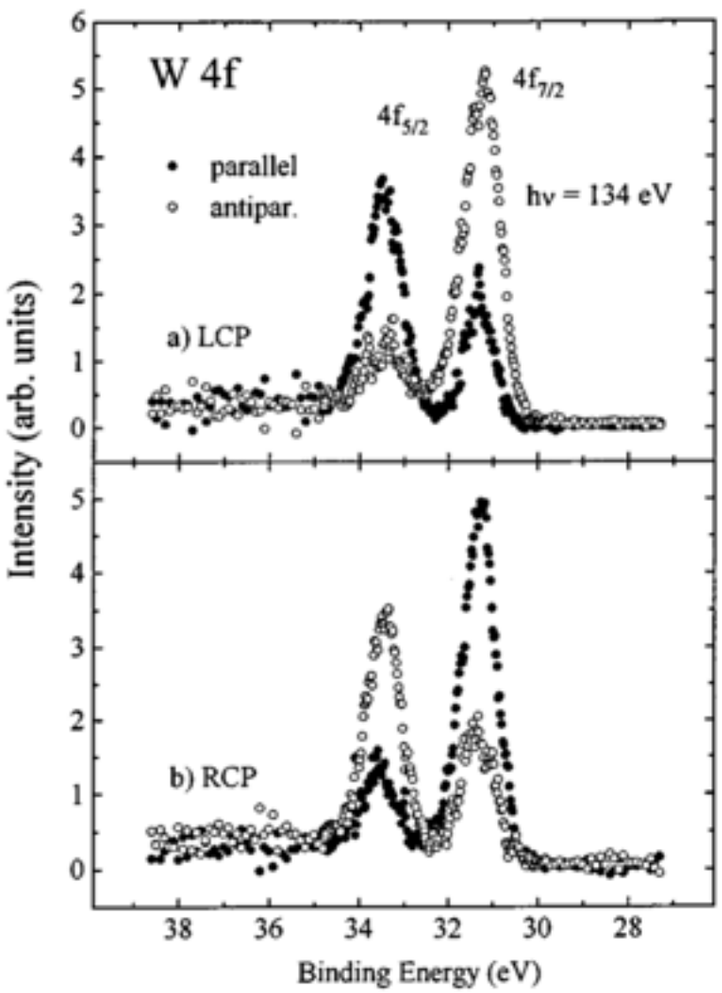
C. Jozwiak *et al.,* Phys. Rev. B 84, 165113 (2011).

Spin signal from Photoemission effect

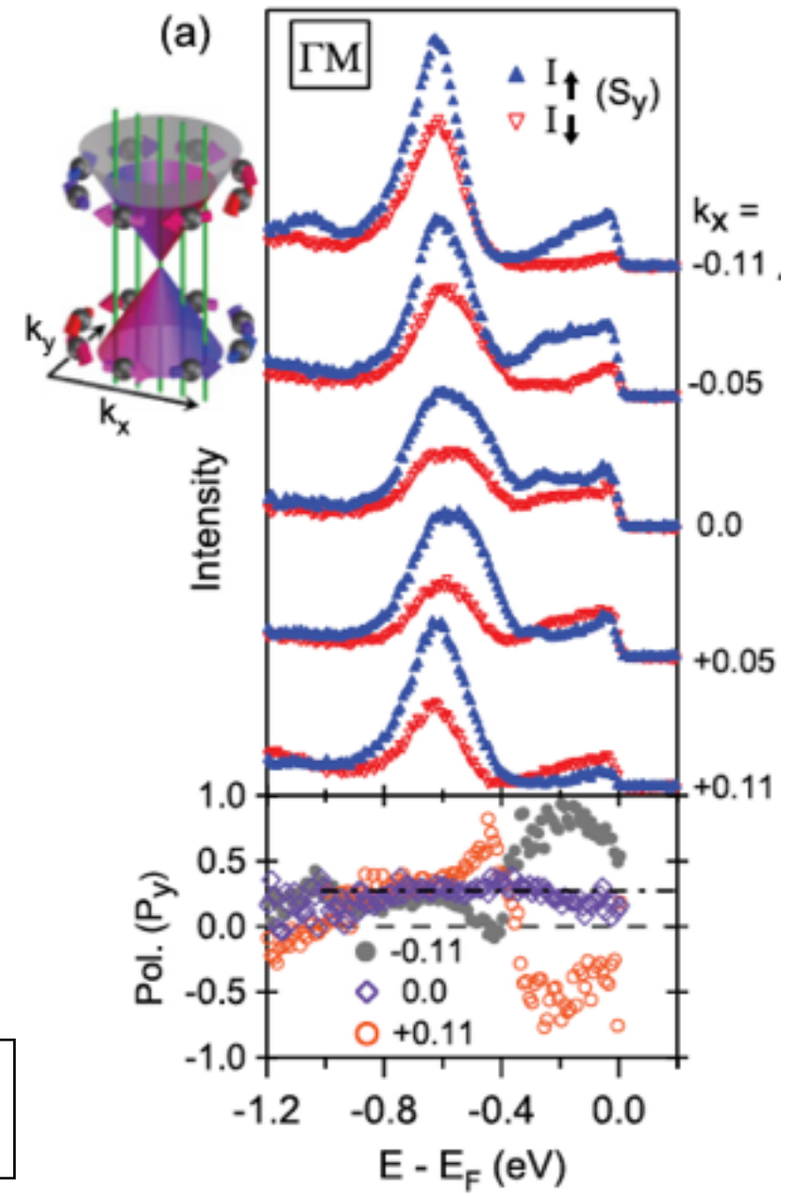
core levels of non-magnetic materials

bulk valence bands of topological insulators

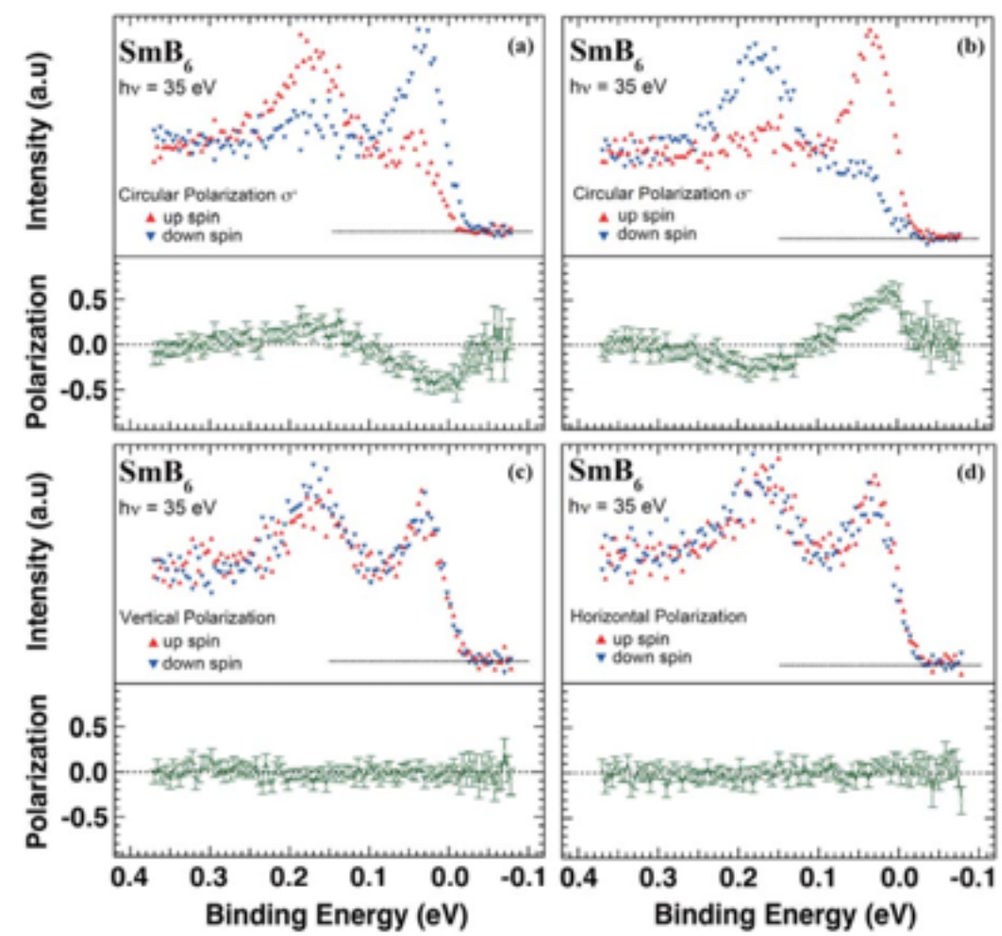
bulk f states of SmB_6



K. Starke *et al.,* Phys. Rev. B 53, 10544 (1996).

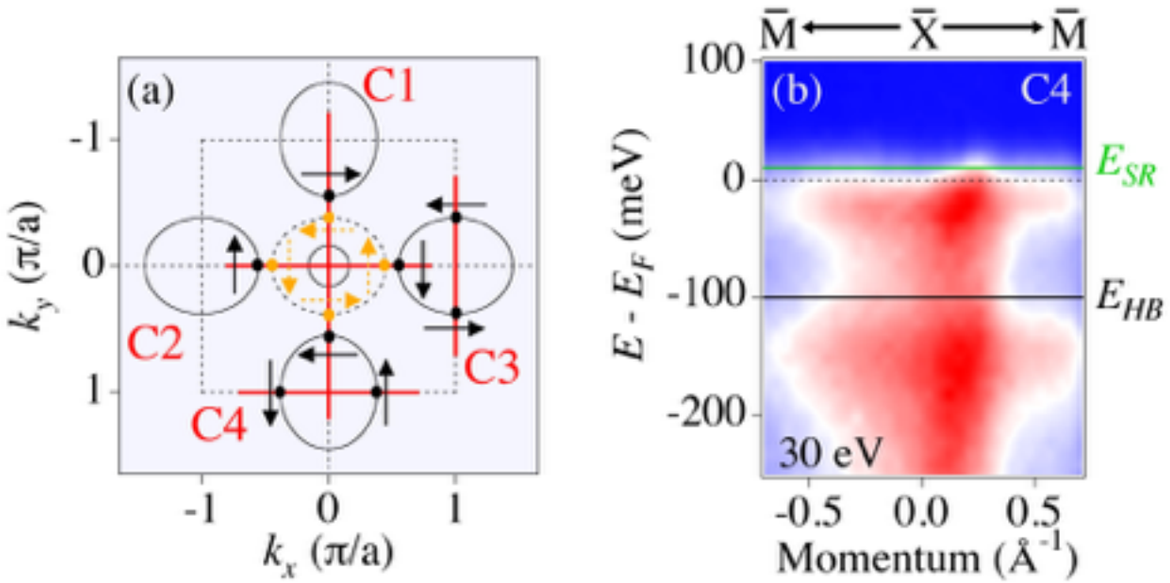


C. Jozwiak *et al.,* Phys. Rev. B 84, 165113 (2011).



S. Suga *et al.,* J. Phys. Soc. Jpn. 83, 014705 (2014).

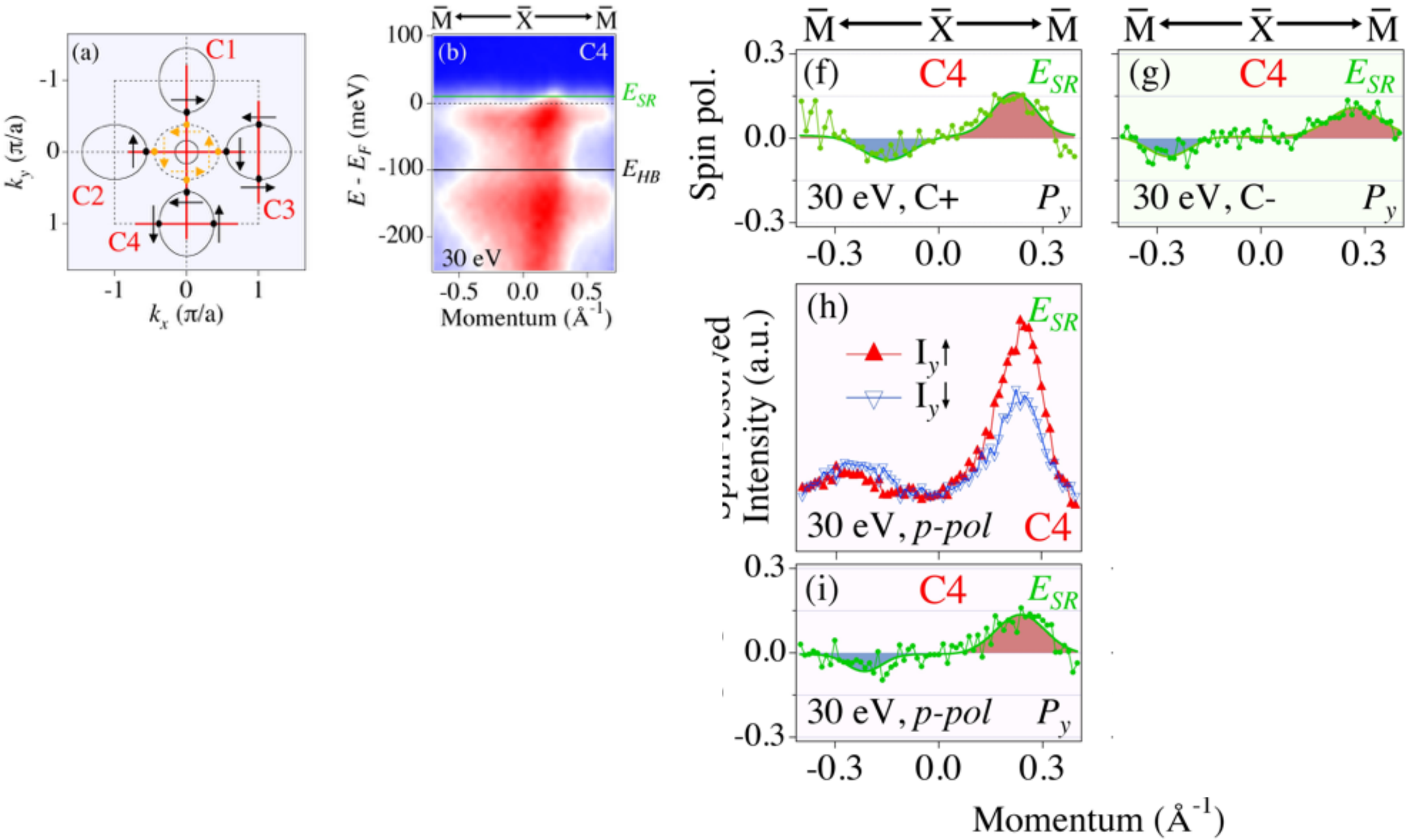
Polarization dependence



Momentum (Å^{-1})

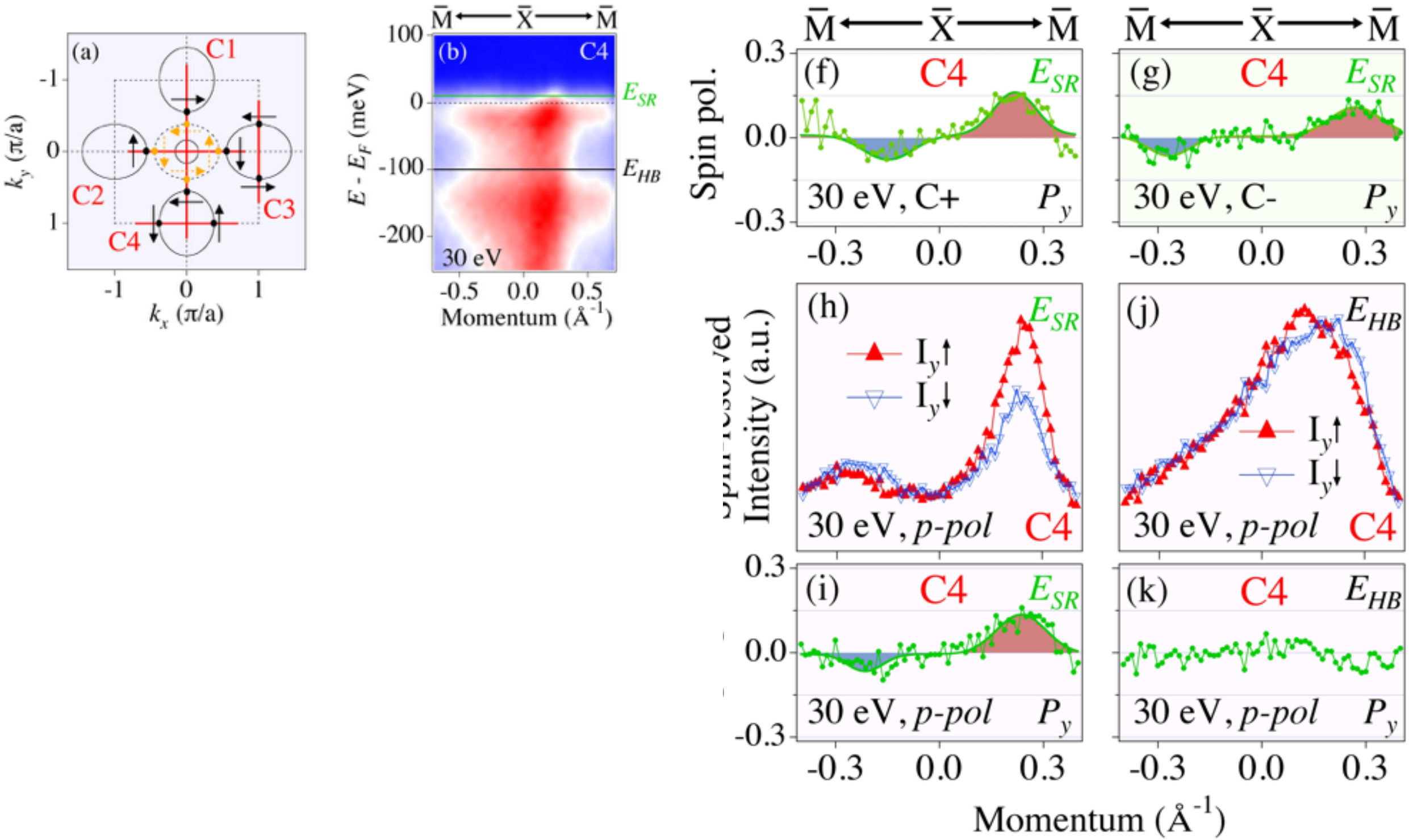
N. Xu *et al*., Nat. Commun. **5**, 4566 (2014).

Polarization dependence



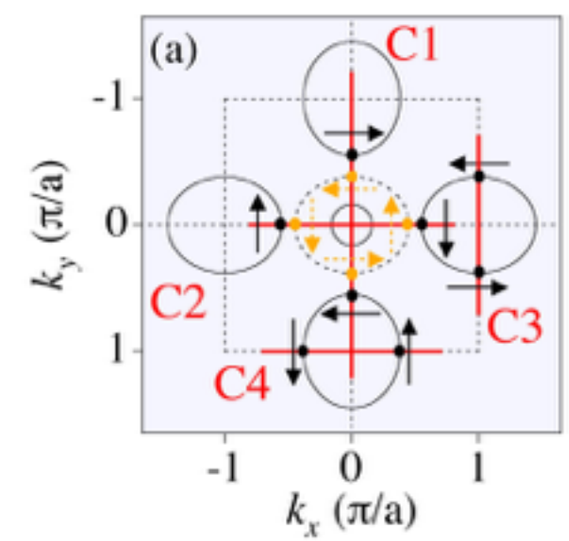
N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

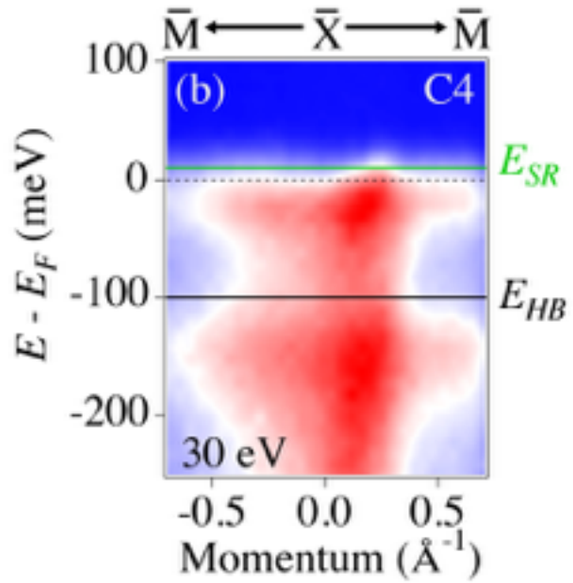
Polarization dependence

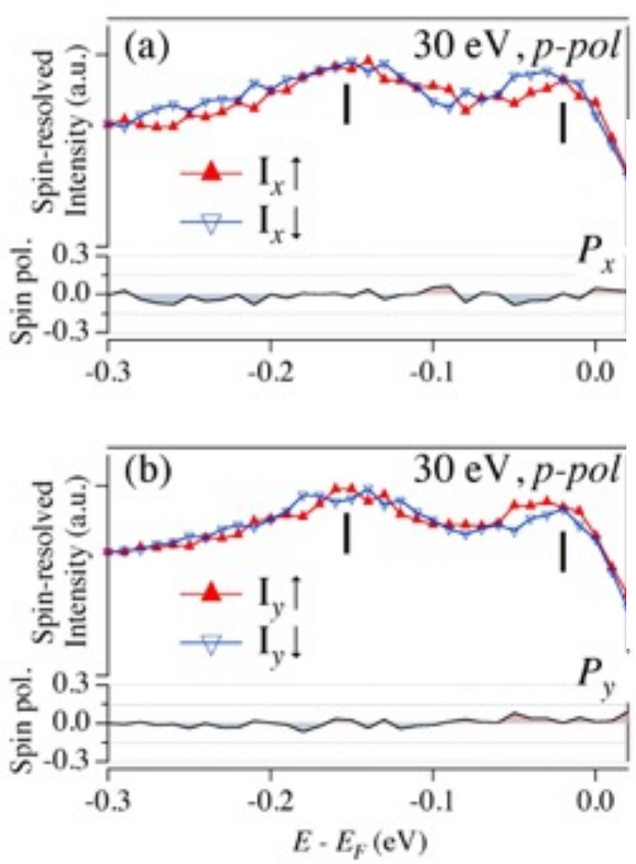


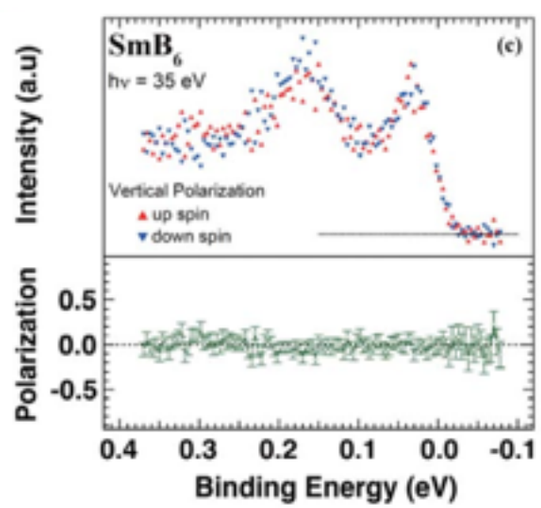
N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

Polarization dependence

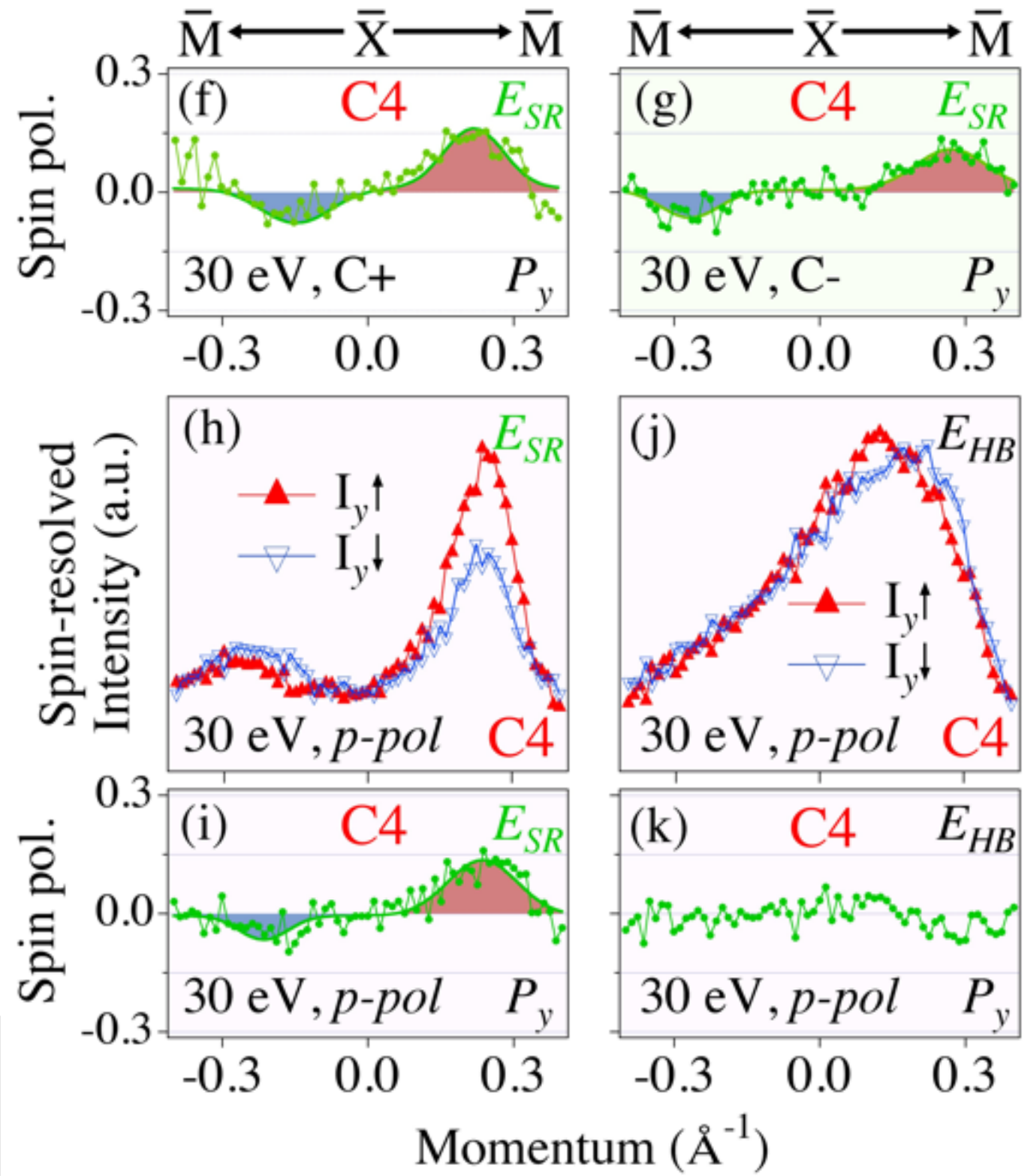






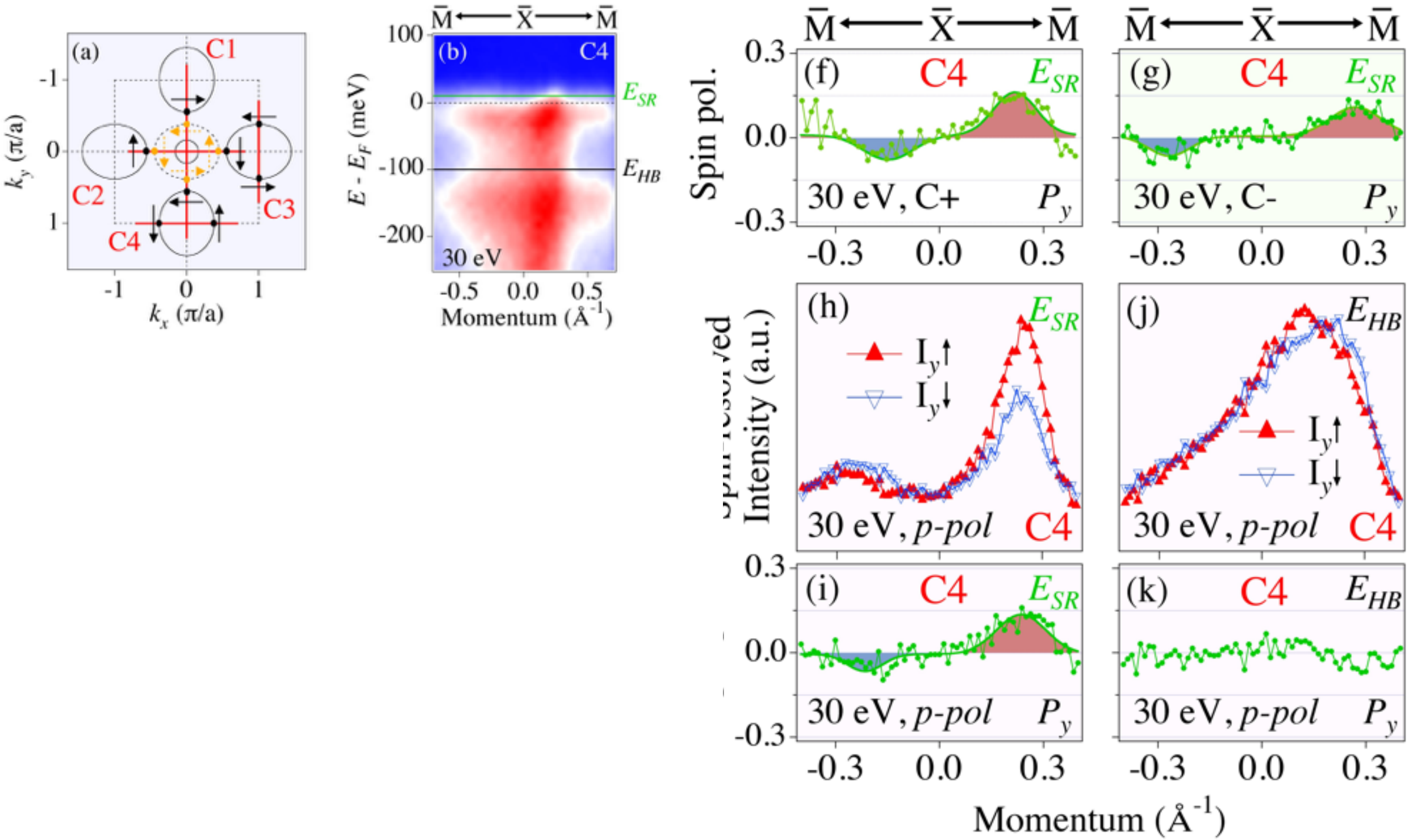


S. Suga *et al.*, J. Phys. Soc. Jpn. 83, 014705 (2014).



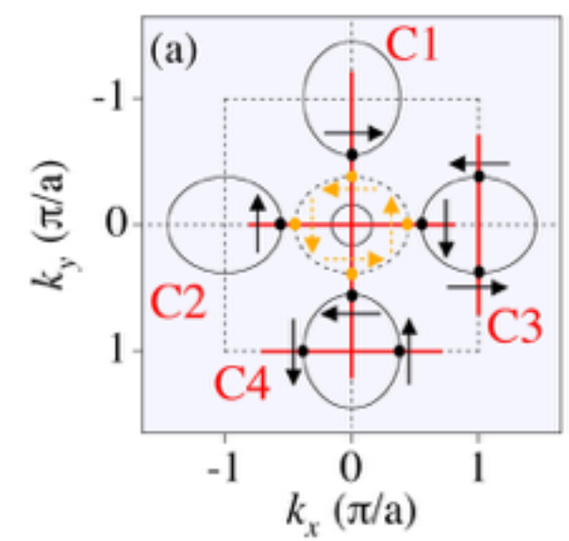
N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

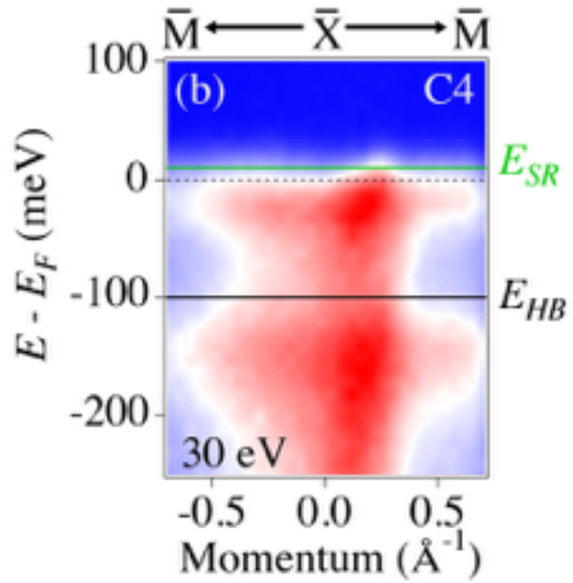
Polarization dependence

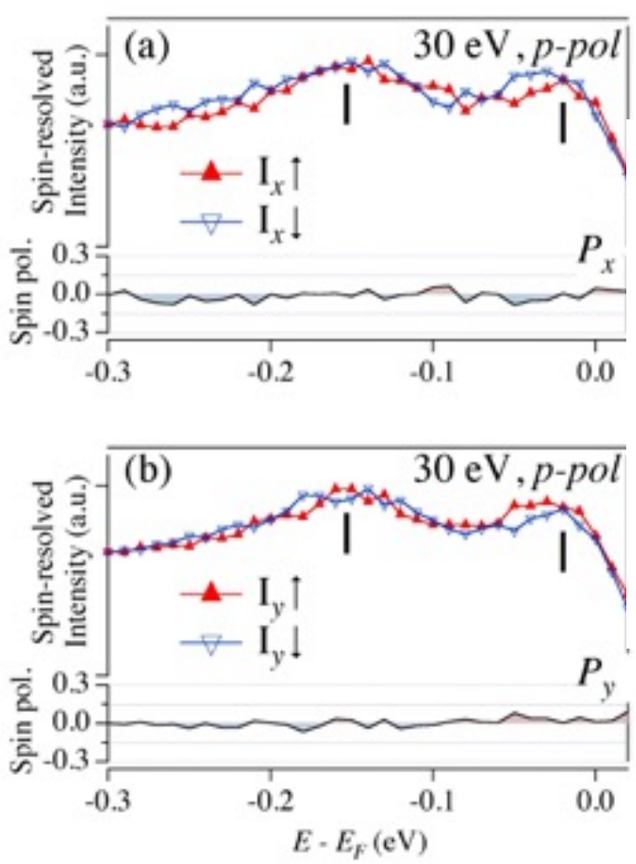


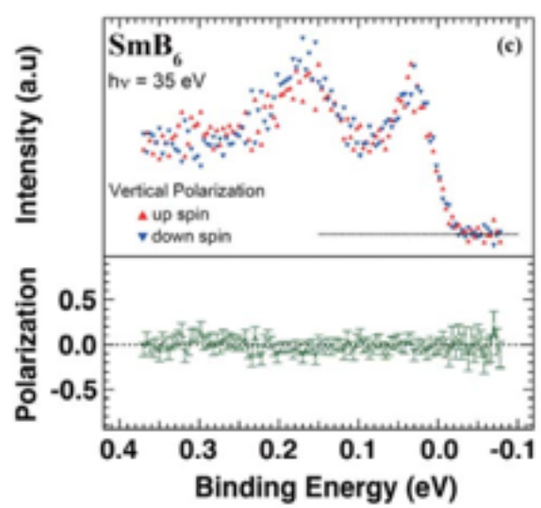
N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

Polarization dependence

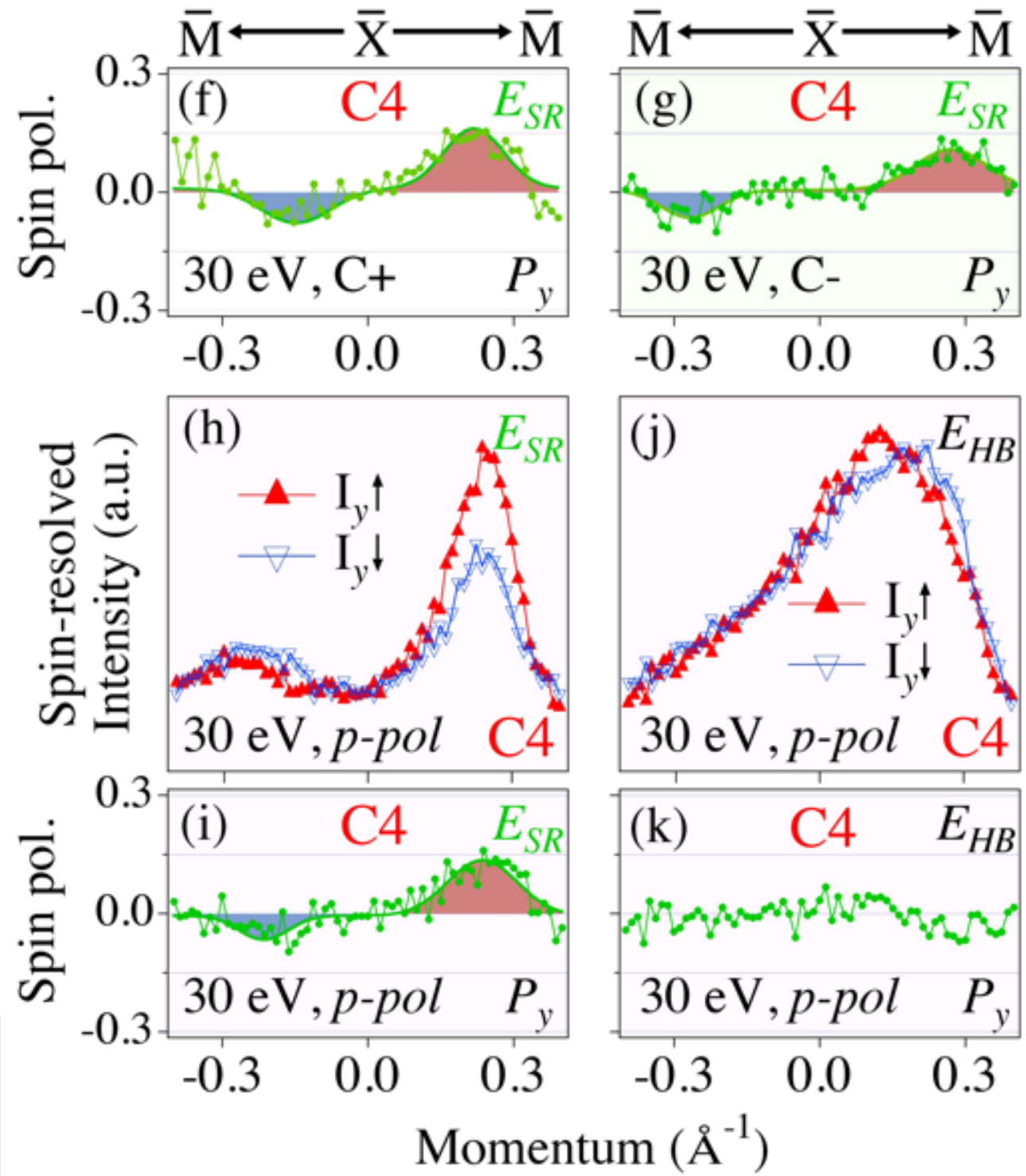






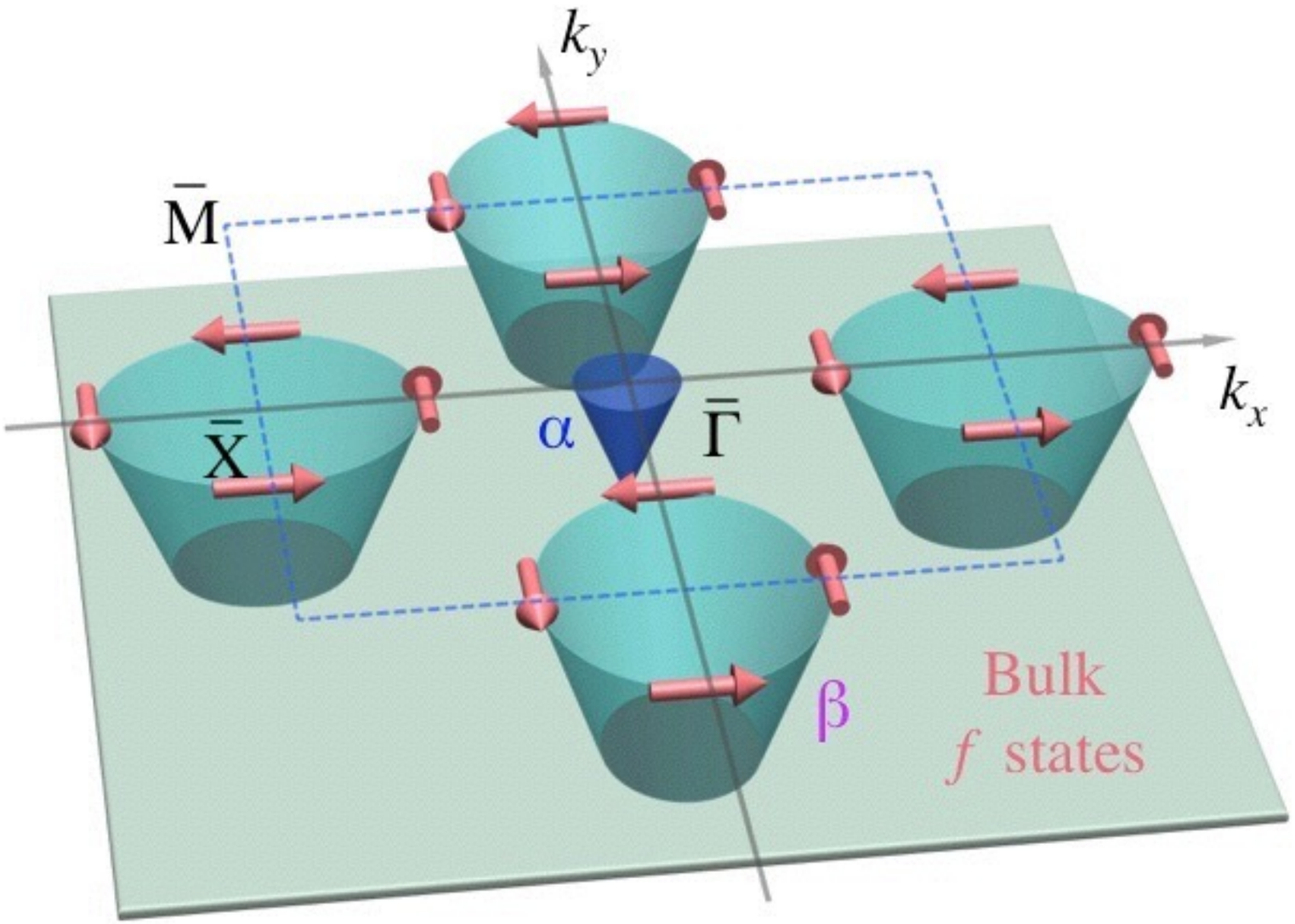


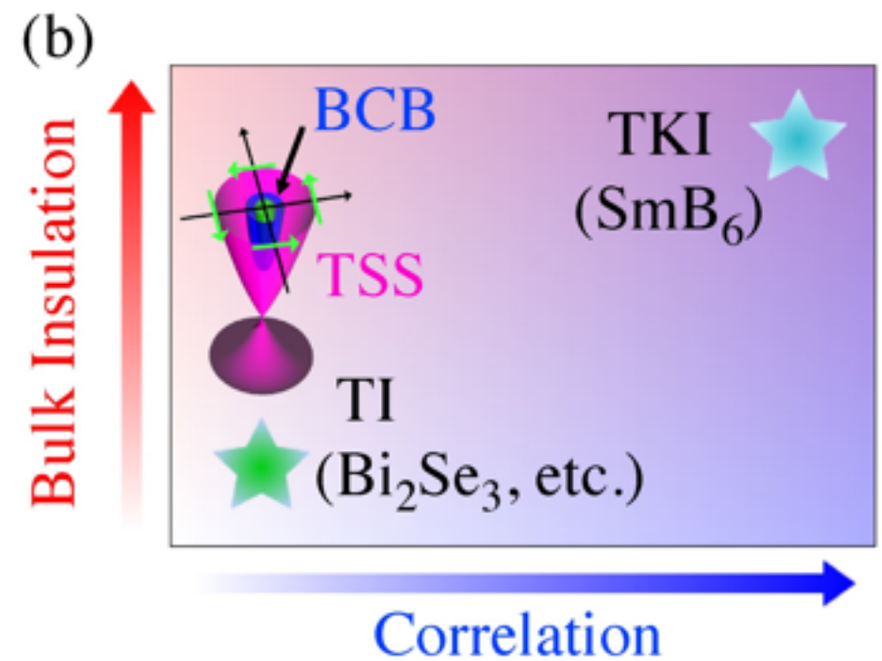
S. Suga *et al.*, J. Phys. Soc. Jpn. 83, 014705 (2014).



N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

Summary

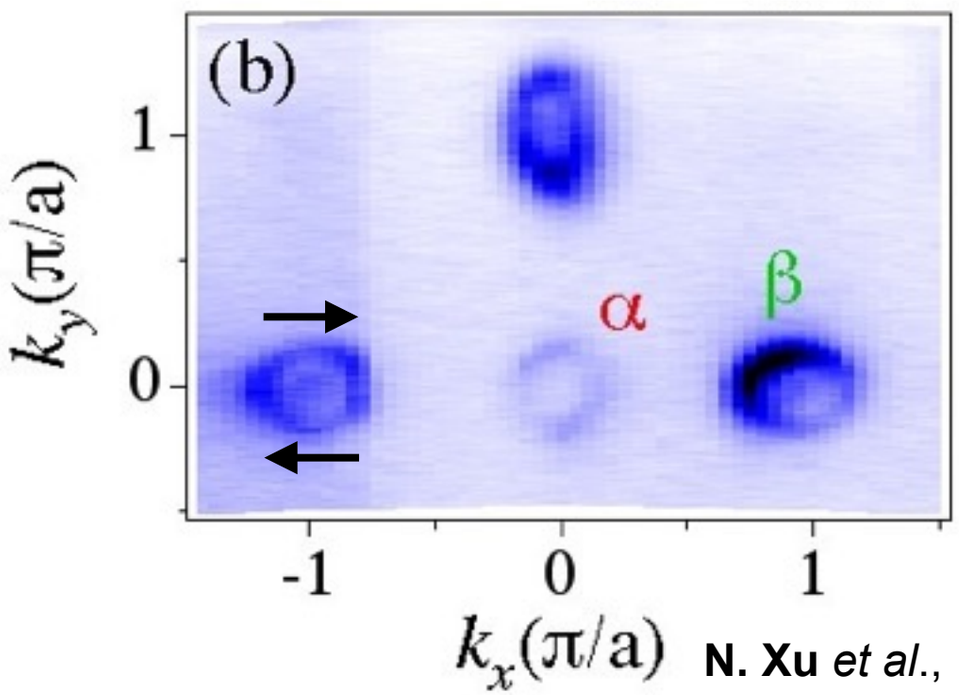




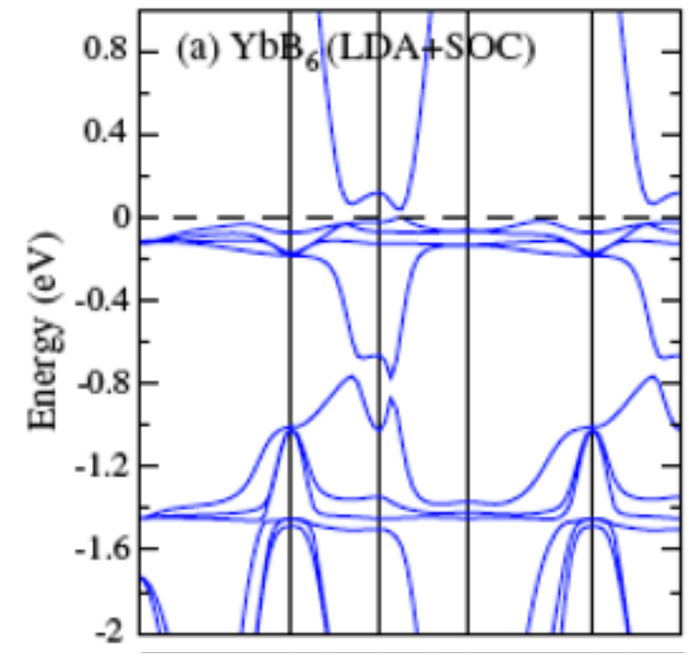
N. Xu *et al.*, Nat. Commun. **5**, 4566 (2014).

Summary

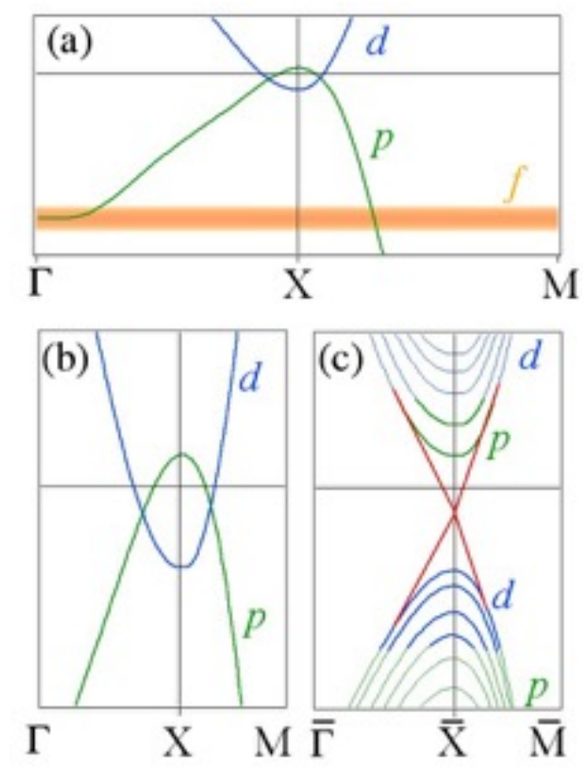
YbB_6



N. Xu *et al.*, arXiv:1405.0165 (2014)

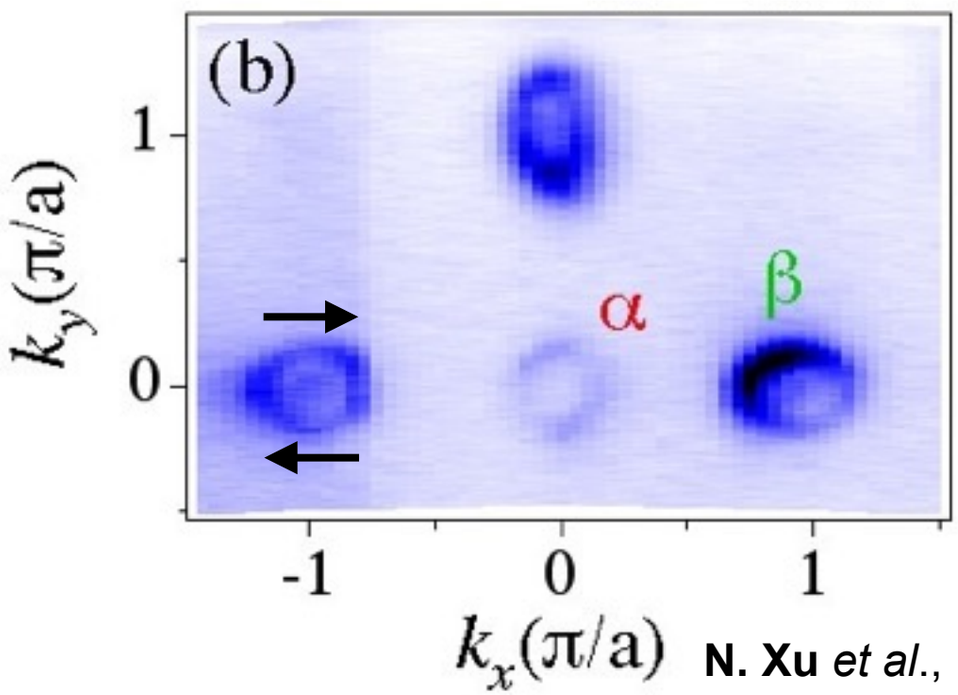


HM Weng, *et al.*, PRL 112, 016403 (2014)

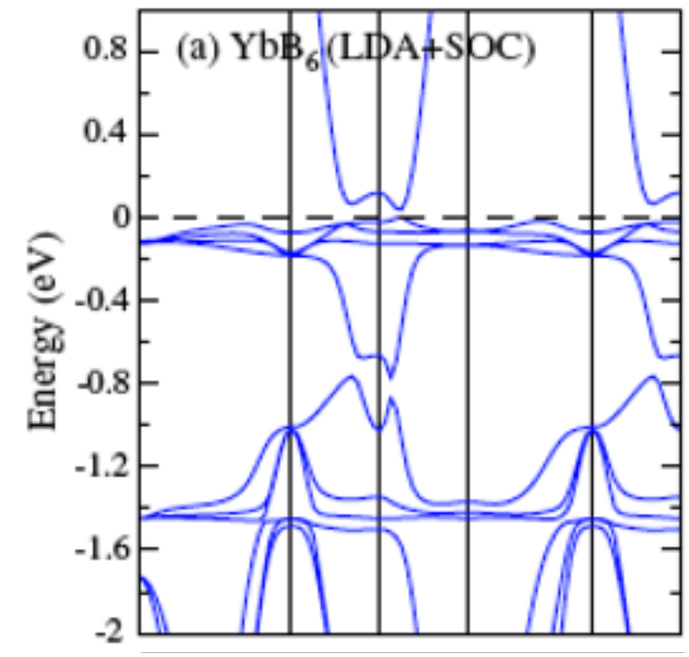


Summary

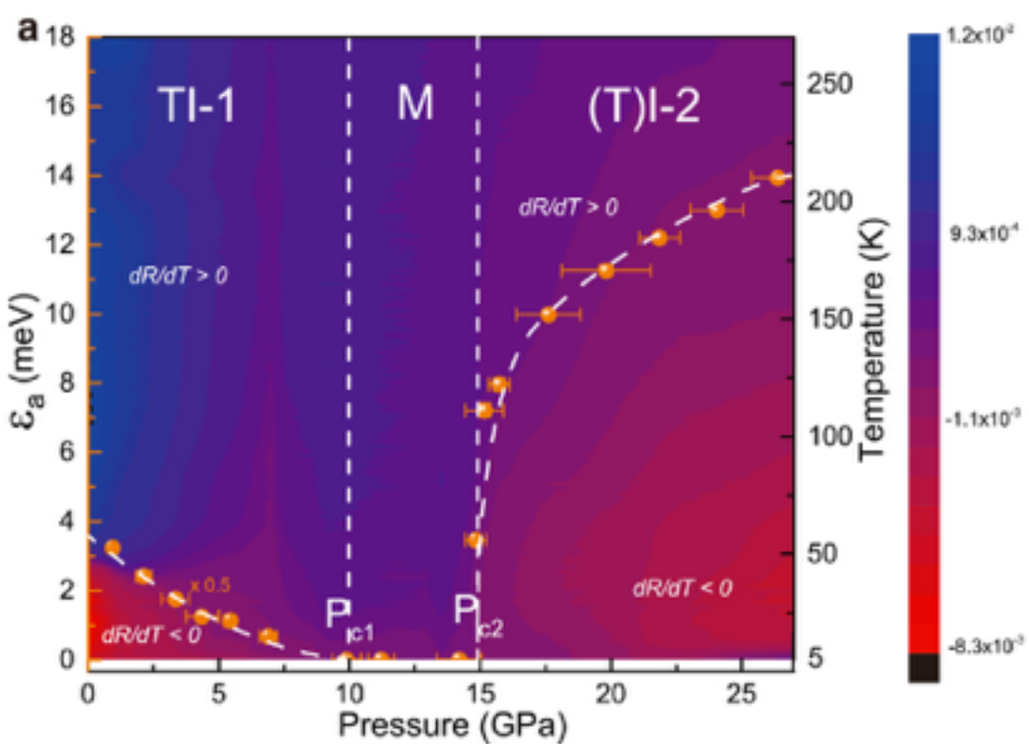
YbB_6



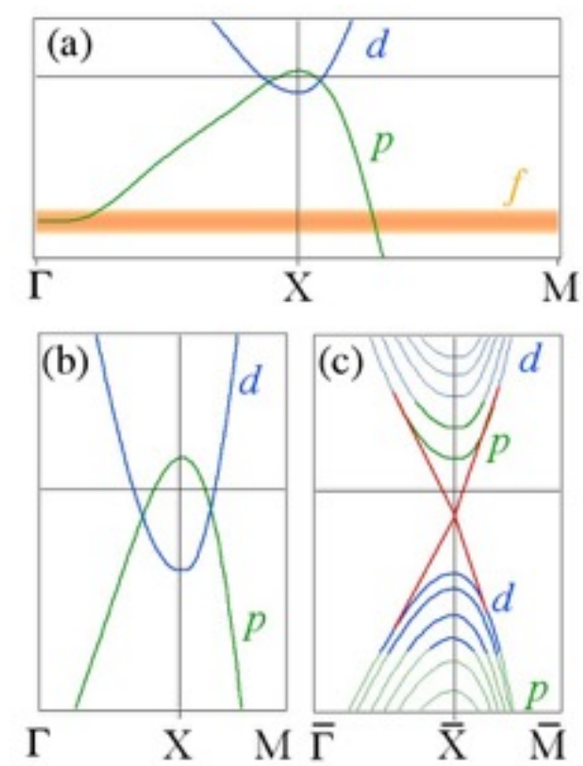
N. Xu *et al.*, arXiv:1405.0165 (2014)



HM Weng, *et al.*, PRL 112, 016403 (2014)



Yazhou Zhou *et al.*, arXiv:1501.03901



Thanks for your attention!